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Algorithm for the Calculation of Absorption Coefficient-Pressure Broadened Molecular Transitions

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FOR THE COMMANDER

John Howard

Chief Scientist

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report describes an algorithm for the accelerated computation of the convolution of a Lorentz line shape (pressure broadened) with spectral line data. A computational savings of approximately 10 has been achieved over conventional methods. The Lorentz function has been decomposed into three functions, each of which is convolved independently at optional sampling intervals. Criteria for the determination of the sampling interval of the Lorentz function for a resultant error of 0.1 percent is described. The report contains

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20. Abstract (Continued)

a listing of the computer program based on the algorithm and sample results in the spectral region 3550 to 3650 cm^{-1} due to water and carbon dioxide.

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Algorithm for the Calculation of Absorption Coefficient-Pressure Broadened Molecular Transitions

1. INTRODUCTION

This report describes an algorithm and associated program to perform the convolution of a line shape function with an array of absorption transitions for which the wavenumber values, the intensities, and the halfwidths are specified. The algorithm has been developed with the objectives of minimizing the number of operations to perform the convolution and of developing a program having reasonable computer storage requirements. The decrease in computational operations achieved by the present method may be utilized to decrease computer time requirements for current problems or, if necessary, to perform more extensive calculations that were not previously considered feasible.

The program described in this report uses a given line shape function (the Lorentz function) which is assumed to be independent of molecular species. The algorithm enables the calculation of the absorption coefficient at equally spaced output wavenumber increments over a specified wavenumber region. A uniform path is assumed for which the temperature, pressure, and absorber amounts are specified. The program has been written to be compatible with the AFGL line listing,[1] and performs the function of program LIN previously utilized in HITRAN

(Received for publication 21 July 1977)

1. McClatchey, R.A., Benedict, W.S., Clough, S.A., Burch, D.E., Calfee, R.F., Fox, K., Rothman, L.S., and Garing, J.S. (1973) AFCRL Atmospheric Absorption Line Parameters Compilation, Report No. AFCRL-TR-73-0096, Environmental Research Papers, No. 434.

calculations. The algorithm has been developed with the goal of keeping the error in the absorption coefficient to within 0.1 percent.

The concept that has been developed involves the decomposition of the given line shape function into three functions which are independently convolved with the parameters for each spectral line. The first function is narrow and describes the central portion of the Lorentzian line shape, the second function is broader describing the intermediate region of the shape, and the third function is broad and may be considered to describe the "near" wing contribution of the line. The functions have been carefully chosen so that the required spectral information is retained as each function is sampled at the same number of points by the convolution process. The spectrum is reconstructed at the final stage by properly interpolating the three functions into the output array of absorption coefficients. Also included in this report is a program that performs a subsequent interpolation providing an essentially continuous resultant spectrum without requiring the convolution calculations to be performed at more output points than are required.

2. DECOMPOSITION OF THE LORENTZ LINE SHAPE

The Lorentz shape is generally applicable for pressure broadened lines for which the transition wavenumber value is large compared to the line halfwidth, and has been discussed by many authors.[2,3,4] The absorption coefficient, $A_i(\nu)$, as a function of wavenumber, ν, resulting from the convolution of the Lorentz line shape with a molecular transition of wavenumber ν_i, intensity S_i, and width α_i (halfwidth at half maximum: HWHM) is given by

$$A_i(\nu) = \frac{S_i}{\pi} \frac{\alpha_i}{\alpha_i^2 + (\nu - \nu_i)^2} = \frac{S_i}{\pi\alpha_i} \frac{1}{1 + \left(\frac{\nu - \nu_i}{\alpha_i}\right)^2} \tag{1}$$

and the total absorption coefficient is given by

$$A(\nu) = \sum_i A_i(\nu) \quad . \tag{2}$$

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2. Goody, R.M. (1964) Atmospheric Radiation I, Theoretical Basis, Oxford, Clarendon Press.

3. Breene, R.B., Jr. (1961) The Shift and Shape and Spectral Lines, Pergamon Press, New York.

4. Mitchell, A.C.G., and Zemansky, M.W. (1934) Resonance Radiation and Excited Atoms, The Macmillan Co., New York.

For computational purposes, it becomes advantageous to define a dimensionless variable z which for a single line is defined as

$$z = \frac{\nu - \nu_l}{\alpha_l} \tag{3}$$

where z is the wavenumber difference from the line center, ν_l, in terms of the halfwidth of the transition. The absorption coefficient for a single line in terms of z is

$$A(z) = \frac{S}{\alpha} \frac{1/\pi}{1 + z^2} = \left(\frac{S}{\alpha}\right) L(z) \tag{4}$$

where the Lorentz function is

$$L(z) = \frac{1/\pi}{1 + z^2} \quad . \tag{5}$$

This definition has the computational advantage that L(z) is explicitly independent of halfwidth and may be tabulated as a numerical function with argument z.

The function L(z) has pathologically slow convergence to zero as has been discussed by Goody[2] and others. In order to avoid computation of the Lorentz function at values of the argument for which the function is slowly varying, the function has been decomposed into three bounded regions ($0 \leq |z| \leq Z_l$, $l = 1, 3$). We have chosen $Z_1 = 3$, $Z_2 = 12$, and $Z_3 = 48$ resulting in three functions with similar functional behavior over the bounds 0 to 3 halfwidths, 0 to 12 halfwidths and 0 to 48 halfwidths respectively.

The decomposition has been performed in a progressive manner by creating the first function (denoted as the "fast function," (XF(z)) as the difference between the Lorentz function and an even quartic function $Q_1(z)$ chosen such that the value, the first derivative and the second derivative of XF(z) are zero at the boundary Z_1. XF(z) is given by

$$XF(z) = 1/\pi\,(L'(z) - Q_1(z)) \quad \textit{for} \quad 0 \leq |z| \leq Z_1 \tag{6}$$

where

$$L'(z) = \pi L(z) = \frac{1}{1 + z^2} \tag{7}$$

$$Q_1(z) = a_1 + b_1 z^2 + c_1 z^4 \tag{8}$$

and

$$c_1 = 1/(1 + Z_b^2)^3 \quad , \quad b_1 = -c_1(1 + 3\,Z_b^2) \quad \text{and} \quad a_1 = c_1(1 + 3\,Z_b^2 + 3\,Z_b^4) \quad . \tag{9}$$

For $Z_b = Z_1 = 3$ we obtain

$$c_1 = \frac{1}{10^3} \quad , \quad b_1 = -\frac{28}{10^3} \quad , \quad \text{and} \quad a_1 = \frac{271}{10^3} \quad . \tag{10}$$

Consequently, we have for the "fast function"

$$XF(z) = 1/\pi\ (1/(1 + z^2) - (a_1 + b_1 z^2 + c_1 z^4) \qquad 0 \le |z| \le 3 \quad , \tag{11}$$

$$XF(z) = 0 \qquad 3 \le |z| \; . \tag{12}$$

The second function, the "slow function," $XS(z)$, is constructed in a similar manner by defining an even quartic function, $Q_2(z)$, in the domain $3 \le |z| \le 12$ which matches the Lorentzian at $z = Z_b = Z_2 = 12$. We obtain by performing operations similar to those above

$$XS(z) = 1/\pi\ (L'(z) - Q_2(z)) \quad \text{for} \quad 3 \le |z| \le 12 \tag{13}$$

with the coefficients for $Q_2(z)$ given by

$$c_2 = \frac{1}{145^3} \quad , \quad b_2 = -433 \cdot c_2 \quad , \quad \text{and} \quad a_2 = 62641 \cdot c_2 \quad . \tag{14}$$

The "slow function" is then defined as

$$XS(z) = 1/\pi\ (Q_1(z) - Q_2(z)) \qquad 0 \le |z| \le 3 \quad , \tag{15}$$

$$XS(z) = 1/\pi\ (1/(1 + z^2) - (a_2 + b_2 z^2 + c_2 z^4)) \qquad 3 \le |z| \le 12 \quad , \tag{16}$$

$$XS(z) = 0 \qquad 12 \le |z| \quad . \tag{17}$$

The third function, the "very slow function," $XVS(z)$, is defined as the Lorentzian for $12 \le |z| \le 48$ and as $Q_2(z)$ for $0 \le |z| \le 12$.

The following tabular form of the decomposition into the respective domains will make the process more clear:

FUNCTION	DOMAIN $0 \le \lvert z \rvert \le 3$	$3 \le \lvert z \rvert \le 12$	$12 \le \lvert z \rvert \le 48$
XF(z)	$\frac{1}{\pi}(L'(z) - Q_1(z))$	0	0
XS(z)	$\frac{1}{\pi}(Q_1(z) - Q_2(z))$	$\frac{1}{\pi}(L'(z) - Q_2(z))$	0
XVS(z)	$\frac{1}{\pi} Q_2(z)$	$\frac{1}{\pi} Q_2(z)$	$\frac{1}{\pi} L'(z)$. (18)

Note that the three functions sum to the Lorentzian in each domain and that the functions are continuous in value, first and second derivative across the boundaries of the domains.

While the choices of the functions and the boundaries may appear to be somewhat arbitrary, an examination of the result demonstrates the advantage of the imposed conditions. Figure 1 is a plot of the three functions from -48 to +48 halfwidths and indicates the dependence of XF(z), XS(z), and XVS(z) as a function of the variable z. It should be noted that 40.71 percent of the integral of the Lorentz function is contained in XF, 42.47 percent in XS, and 15.50 percent in XVS. The remaining 1.32 percent is outside the 48 halfwidth cutoff.

The three functions are represented in Figure 2 with the horizontal axis determined by the boundary of each function and the vertical axis chosen appropriately for each function. The three functions in this representation are seen to be functionally similar and as a consequence, it is possible to sample each function at the same sampling interval to perform the convolution. One hundred and fifty one (151) values of each symmetric function are stored in the computer program, and it is these values that are plotted in Figure 2 as indicated by the index on the top horizontal axis. The tabulation of this number of values for the functions precludes the necessity for interpolation in the convolution calculation. The values of the functions are tabulated in Table 1.

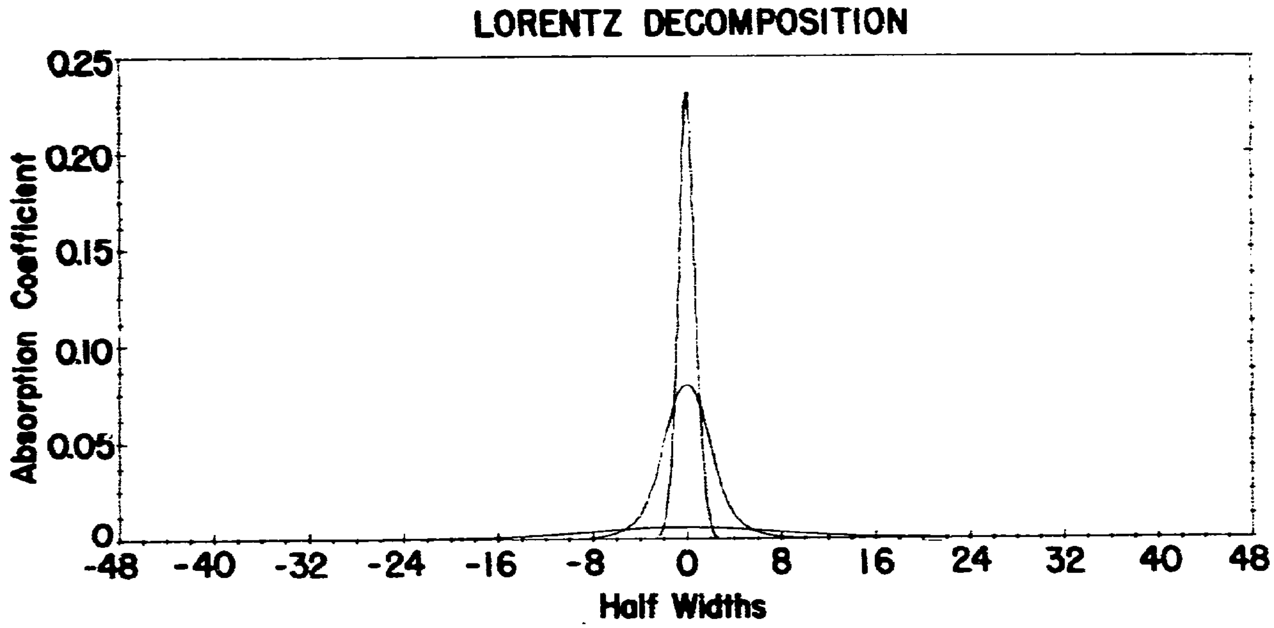

Figure 1. Decomposition of the Lorentz Function into Three Domains: -3 to 3 halfwidths, -12 to 12 halfwidths and -48 to 48 halfwidths. The sum of the three functions gives $L(z) = (1/\pi)(1/1 + z^2)$

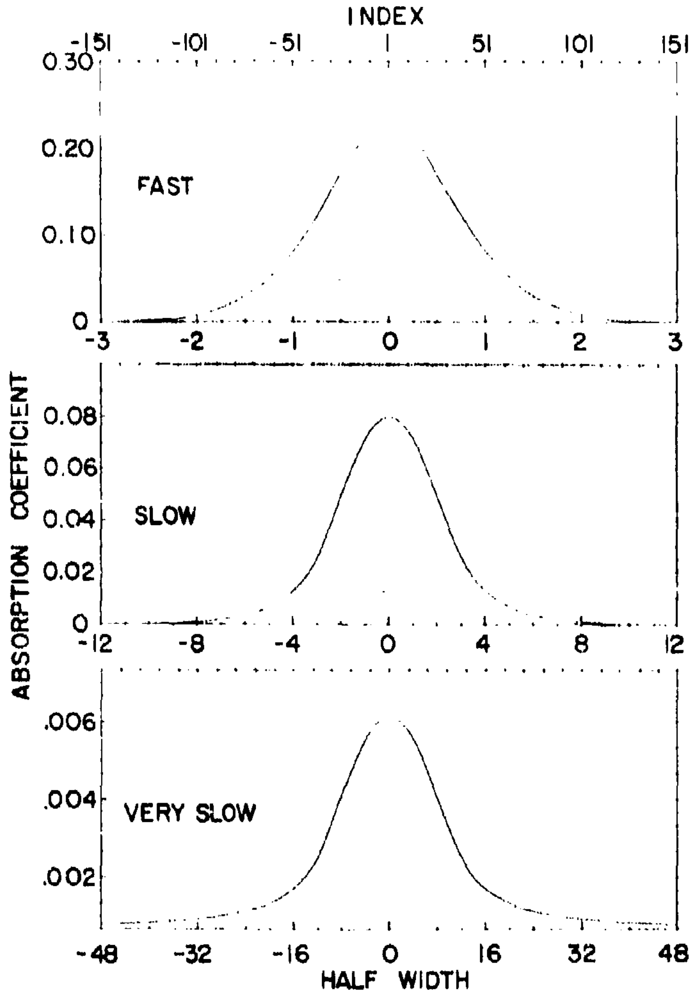

Figure 2. Functional Behavior of the Decomposed Functions Over Their Respective Limits. Plots are direct plots of the functions in terms of the storage index of the program. The fast function (XF) is on the top, the slow function (XS) is in the middle, and the very slow functions (XVS) are on the bottom

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α, that is, $z = |(\nu - \nu_o)/\alpha|$. Plots of the three tabulated functions appear in Figure 2 and Figure 3

INDEX	Z	"FAST" FUNCTION FN	Z	"SLOW" FUNCTION FN	Z	"VERY SLOW" FUNCTION FN
1	0.000	2.320E-01	0.000	7.972E-02	0.000	6.540E-03
2	.020	2.319E-01	.080	7.966E-02	.320	6.536E-03
3	.040	2.316E-01	.160	7.949E-02	.640	6.522E-03
4	.060	2.309E-01	.240	7.921E-02	.960	6.499E-03
5	.080	2.301E-01	.320	7.882E-02	1.280	6.467E-03
6	.100	2.290E-01	.400	7.831E-02	1.600	6.425E-03
7	.120	2.277E-01	.480	7.770E-02	1.920	6.375E-03
8	.140	2.261E-01	.560	7.697E-02	2.240	6.316E-03
9	.160	2.243E-01	.640	7.614E-02	2.560	6.249E-03
10	.180	2.223E-01	.720	7.521E-02	2.880	6.173E-03
11	.200	2.202E-01	.800	7.418E-02	3.200	6.088E-03
12	.220	2.178E-01	.880	7.305E-02	3.520	5.996E-03
13	.240	2.152E-01	.960	7.182E-02	3.840	5.896E-03
14	.260	2.125E-01	1.040	7.050E-02	4.160	5.789E-03
15	.280	2.096E-01	1.120	6.910E-02	4.480	5.675E-03
16	.300	2.066E-01	1.200	6.761E-02	4.800	5.554E-03
17	.320	2.034E-01	1.280	6.605E-02	5.120	5.427E-03
18	.340	2.001E-01	1.360	6.441E-02	5.440	5.294E-03
19	.360	1.967E-01	1.440	6.270E-02	5.760	5.155E-03
20	.380	1.932E-01	1.520	6.093E-02	6.080	5.012E-03
21	.400	1.896E-01	1.600	5.911E-02	6.400	4.864E-03
22	.420	1.859E-01	1.680	5.723E-02	6.720	4.712E-03
23	.440	1.821E-01	1.760	5.531E-02	7.040	4.556E-03
24	.460	1.783E-01	1.840	5.335E-02	7.360	4.398E-03
25	.480	1.745E-01	1.920	5.136E-02	7.680	4.237E-03
26	.500	1.706E-01	2.000	4.934E-02	8.000	4.075E-03
27	.520	1.667E-01	2.080	4.731E-02	8.320	3.911E-03
28	.540	1.628E-01	2.160	4.528E-02	8.640	3.747E-03
29	.560	1.588E-01	2.240	4.324E-02	8.960	3.584E-03
30	.580	1.549E-01	2.320	4.121E-02	9.280	3.421E-03
31	.600	1.510E-01	2.400	3.920E-02	9.600	3.261E-03
32	.620	1.470E-01	2.480	3.722E-02	9.920	3.103E-03
33	.640	1.432E-01	2.560	3.527E-02	10.240	2.948E-03
34	.660	1.393E-01	2.640	3.338E-02	10.560	2.797E-03
35	.680	1.355E-01	2.720	3.153E-02	10.880	2.652E-03
36	.700	1.317E-01	2.800	2.976E-02	11.200	2.512E-03
37	.720	1.279E-01	2.880	2.806E-02	11.520	2.379E-03
38	.740	1.242E-01	2.960	2.646E-02	11.840	2.255E-03
39	.760	1.205E-01	3.040	2.495E-02	12.160	2.138E-03
40	.780	1.169E-01	3.120	2.354E-02	12.480	2.031E-03
41	.800	1.134E-01	3.200	2.223E-02	12.800	1.931E-03
42	.820	1.099E-01	3.280	2.100E-02	13.120	1.839E-03
43	.840	1.065E-01	3.360	1.966E-02	13.440	1.752E-03
44	.860	1.031E-01	3.440	1.878E-02	13.760	1.672E-03
45	.880	9.984E-02	3.520	1.778E-02	14.080	1.598E-03
46	.900	9.661E-02	3.600	1.683E-02	14.400	1.528E-03
47	.920	9.345E-02	3.680	1.594E-02	14.720	1.462E-03
48	.940	9.035E-02	3.760	1.511E-02	15.040	1.401E-03
49	.960	8.733E-02	3.840	1.432E-02	15.360	1.343E-03
50	.980	8.437E-02	3.920	1.358E-02	15.680	1.289E-03
51	1.000	8.149E-02	4.000	1.288E-02	16.000	1.239E-03
52	1.020	7.867E-02	4.080	1.222E-02	16.320	1.191E-03
53	1.040	7.592E-02	4.160	1.160E-02	16.640	1.145E-03
54	1.060	7.324E-02	4.240	1.101E-02	16.960	1.103E-03
55	1.080	7.063E-02	4.320	1.046E-02	17.280	1.062E-03
56	1.100	6.809E-02	4.400	9.930E-03	17.600	1.024E-03
57	1.120	6.561E-02	4.480	9.432E-03	17.920	9.882E-04
58	1.140	6.320E-02	4.560	8.960E-03	18.240	9.539E-04
59	1.160	6.086E-02	4.640	8.513E-03	18.560	9.214E-04
60	1.180	5.858E-02	4.720	8.089E-03	18.880	8.909E-04

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α, that is, $z = |(\nu - \nu_0)/\alpha|$. Plots of the three tabulated functions appear in Figure 2 and Figure 3 (Cont.)

INDEX	"FAST" FUNCTION Z	"FAST" FUNCTION FN	"SLOW" FUNCTION Z	"SLOW" FUNCTION FN	"VERY SLOW" FUNCTION Z	"VERY SLOW" FUNCTION FN
61	1.200	5.637E-02	4.800	7.687E-03	19.200	8.611E-04
62	1.220	5.422E-02	4.880	7.305E-03	19.520	8.332E-04
63	1.240	5.213E-02	4.960	6.942E-03	19.840	8.066E-04
64	1.760	5.010E-02	5.040	6.597E-03	20.160	7.813E-04
65	1.280	4.813E-02	5.120	6.269E-03	20.480	7.571E-04
66	1.300	4.622E-02	5.200	5.958E-03	20.800	7.340E-04
67	1.320	4.437E-02	5.280	5.661E-03	21.120	7.120E-04
68	1.340	4.258E-02	5.360	5.379E-03	21.440	6.910E-04
69	1.360	4.084E-02	5.440	5.111E-03	21.760	6.708E-04
70	1.380	3.915E-02	5.520	4.855E-03	22.080	6.516E-04
71	1.400	3.752E-02	..600	4.611E-03	22.400	6.331E-04
72	1.420	3.594E-02	5.680	4.379E-03	22.720	6.155E-04
73	1.440	3.441E-02	5.760	4.158E-03	23.040	5.985E-04
74	1.460	3.293E-02	5.840	3.947E-03	23.360	5.822E-04
75	1.480	3.150E-02	5.920	3.746E-03	23.680	5.666E-04
76	1.500	3.012E-02	6.000	3.555E-03	24.000	5.517E-04
77	1.520	2.879E-02	6.080	3.372E-03	24.320	5.373E-04
78	1.540	2.749E-02	6.160	3.198E-03	24.640	5.234E-04
79	1.560	2.625E-02	6.240	3.032E-03	24.960	5.101E-04
80	1.580	2.504E-02	6.320	2.873E-03	25.280	4.973E-04
81	1.600	2.388E-02	6.400	2.722E-03	25.600	4.850E-04
82	1.620	2.276E-02	6.480	2.578E-03	25.920	4.731E-04
83	1.640	2.168E-02	6.560	2.441E-03	26.240	4.616E-04
84	1.660	2.064E-02	6.640	2.309E-03	26.560	4.506E-04
85	1.680	1.963E-02	6.720	2.184E-03	26.880	4.399E-04
86	1.700	1.866E-02	6.800	2.065E-03	27.200	4.297E-04
87	1.720	1.773E-02	6.880	1.951E-03	27.520	4.197E-04
88	1.740	1.684E-02	6.960	1.843E-03	27.840	4.102E-04
89	1.760	1.597E-02	7.040	1.739E-03	28.160	4.009E-04
90	1.780	1.514E-02	7.120	1.641E-03	28.480	3.920E-04
91	1.800	1.435E-02	7.200	1.547E-03	28.800	3.833E-04
92	1.820	1.358E-02	7.280	1.457E-03	29.120	3.749E-04
93	1.840	1.284E-02	7.360	1.372E-03	29.440	3.668E-04
94	1.860	1.214E-02	7.440	1.291E-03	29.760	3.590E-04
95	1.680	1.146E-02	7.520	1.213E-03	30.080	3.514E-04
96	1.900	1.081E-02	7.600	1.140E-03	30.400	3.441E-04
97	1.920	1.019E-02	7.680	1.070E-03	30.720	3.369E-04
98	1.940	9.594E-03	7.760	1.003E-03	31.040	3.300E-04
99	1.960	9.024E-03	7.840	9.397E-04	31.360	3.233E-04
100	1.980	8.479E-03	7.920	8.796E-04	31.680	3.164E-04
101	2.000	7.958E-03	8.000	8.224E-04	32.000	3.105E-04
102	2.020	7.460E-03	8.080	7.682E-04	32.320	3.044E-04
103	2.040	6.985E-03	8.160	7.167E-04	32.640	2.985E-04
104	2.060	6.532E-03	8.240	6.679E-04	32.960	2.927E-04
105	2.080	6.101E-03	8.320	6.217E-04	33.280	2.871E-04
106	2.100	5.690E-03	8.400	5.779E-04	33.600	2.817E-04
107	2.120	5.299E-03	8.480	5.365E-04	33.920	2.764E-04
108	2.140	4.928E-03	8.560	4.973E-04	34.240	2.713E-04
109	2.160	4.575E-03	8.640	4.603E-04	34.560	2.663E-04
110	2.180	4.241E-03	8.720	4.254E-04	34.880	2.614E-04
111	2.200	3.924E-03	8.800	3.925E-04	35.200	2.567E-04
112	2.220	3.624E-03	8.880	3.615E-04	35.520	2.521E-04
113	2.240	3.341E-03	8.960	3.323E-04	35.840	2.476E-04
114	2.260	3.073E-03	9.040	3.049E-04	36.160	2.433E-04
115	2.280	2.821E-03	9.120	2.791E-04	36.480	2.390E-04
116	2.300	2.584E-03	9.200	2.550E-04	36.800	2.349E-04
117	2.320	2.361E-03	9.280	2.324E-04	37.120	2.308E-04
118	2.340	2.152E-03	9.360	2.113E-04	37.440	2.269E-04
119	2.360	1.956E-03	9.440	1.916E-04	37.760	..231E-04
120	2.380	1.773E-03	9.520	1.732E-04	38.080	2.194E-04

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α, that is, $z = |(\nu - \nu_0)/\alpha|$. Plots of the three tabulated functions appear in Figure 2 and Figure 3 (Cont.)

INDEX	"FAST" FUNCTION Z	"FAST" FUNCTION FN	"SLOW" FUNCTION Z	"SLOW" FUNCTION FN	"VERY SLOW" FUNCTION Z	"VERY SLOW" FUNCTION FN
121	2.400	1.602E-03	9.600	1.561E-04	38.400	2.157E-04
122	2.420	1.442E-03	9.680	1.403E-04	38.720	2.122E-04
123	2.440	1.294E-03	9.760	1.256E-04	39.040	2.087E-04
124	2.460	1.157E-03	9.840	1.121E-04	39.360	2.053E-04
125	2.480	1.030E-03	9.920	9.955E-05	39.680	2.020E-04
126	2.500	9.131E-04	10.000	8.806E-05	40.000	1.988E-04
127	2.520	8.055E-04	10.080	7.753E-05	40.320	1.957E-04
128	2.540	7.070E-04	10.160	6.791E-05	40.640	1.926E-04
129	2.560	6.170E-04	10.240	5.915E-05	40.960	1.896E-04
130	2.580	5.352E-04	10.320	5.121E-05	41.280	1.867E-04
131	2.600	4.610E-04	10.400	4.403E-05	41.600	1.838E-04
132	2.620	3.942E-04	10.480	3.758E-05	41.920	1.810E-04
133	2.640	3.343E-04	10.560	3.182E-05	42.240	1.783E-04
134	2.660	2.809E-04	10.640	2.669E-05	42.560	1.756E-04
135	2.680	2.336E-04	10.720	2.215E-05	42.880	1.730E-04
136	2.700	1.920E-04	10.800	1.818E-05	43.200	1.705E-04
137	2.720	1.557E-04	10.880	1.472E-05	43.520	1.680E-04
138	2.740	1.244E-04	10.960	1.174E-05	43.840	1.655E-04
139	2.760	9.758E-05	11.040	9.194E-06	44.160	1.631E-04
140	2.780	7.498E-05	11.120	7.054E-06	44.480	1.608E-04
141	2.800	5.620E-05	11.200	5.280E-06	44.800	1.585E-04
142	2.820	4.088E-05	11.280	3.834E-06	45.120	1.563E-04
143	2.840	2.865E-05	11.360	2.653E-06	45.440	1.541E-04
144	2.860	1.915E-05	11.440	1.791E-06	45.760	1.519E-04
145	2.880	1.203E-05	11.520	1.124E-06	46.080	1.498E-04
146	2.900	6.947E-06	11.600	6.479E-07	46.400	1.478E-04
147	2.920	3.549E-06	11.680	3.306E-07	46.720	1.458E-04
148	2.940	1.494E-06	11.760	1.390E-07	47.040	1.438E-04
149	2.960	4.418E-07	11.840	4.104E-08	47.360	1.419E-04
150	2.980	5.511E-08	11.920	5.113E-09	47.680	1.400E-04
151	3.000	0.	12.000	0.	48.000	1.381E-04

The rationalization for terminating the convolution at 48 halfwidths is based on three considerations: (1) evidence that the line shape deviates from Lorentz behavior for $(\nu - \nu_0)$ of the order of 5 cm^{-1}, corresponding to $z \approx 48$ for a typical atmospheric line at atmospheric pressure (Winters et al;[5] Holstein;[6] Breene;[3] Burch;[7]) (2) the value of the Lorentzian at 48 halfwidths is 1.38×10^{-4} which is

5. Winters, B.H., Silverman, S., and Benedict, W.S. (1964) Line shape in the wing beyond the band head of the 4.3 μ band of CO_2, J. Quant. Spect. Rad. Trans. 4:527.

6. Holstein, T. (1950) Pressure broadening of spectral lines, Phys. Rev. 79:744; see also L. Spitzer Phys. Rev. 58:348 (1940).

7. Burch, D.E., Grynak, D.A., Patty, R.R. and Bartky, C.E. (1968) The Shapes of Collision Broadened CO_2 Lines, Philco Ford Corp., Aeronutronic Report U-3203.

sufficiently small for most calculations, and (3) calculation beyond 48 halfwidths requires an unwarranted increase in computational effort. Although the value of the Lorentz function may justify termination of the calculation at 48 halfwidths, it must not be forgotten that 1.32 percent of the integrated absorption is beyond this region. This is a result of the previously mentioned slow convergence of $1/z^2$ (Goody,[2] and Townes and Schawlow[8]). It is suggested that calculations of the far wings of the lines can more appropriately be done in a parametrized tabulation of what is currently referred to as the continuum for each of the molecular species of interest. The contribution of this continuum function to the absorption coefficient may be calculated at large sampling intervals in the wavenumber domain with negligible effect on computational time.

3. SAMPLING INTERVAL

General discussions of the proper choice of the sampling interval appear in the literature for the type of "line by line" calculations described in this report.[9, 10, 11, 12] These references are primarily concerned with the effect of the sampling interval on the integral of the absorption coefficient or absorptance over a specified wavenumber interval. That approach is particularly appropriate to the case in which an instrumental scanning function that is broad compared to the spectral line widths, is being convolved with the true line spectrum. The present discussion is concerned with the development of a quantitative evaluation of the error introduced in the reconstruction of the spectrum in the interval between sampled points.

An approach that provides direct insight into the problem of determining the sampling interval is that obtained from information theory and the Nyquist sampling theorem. Simple and readily comprehensible discussions of this are provided by

8. Townes, C.H., and Schawlow, A.L. (1955) Microwave Spectroscopy, McGraw Hill-Book Co., New York.

9. Drayson, D.R. (1967) The Calculation of Long Wave Radiative Transfer in Planetary Atmospheres, Report No. 07584-1-T, University of Michigan, Ann Arbor.

10. Kyle, T.G. (1968) Net interval for calculating absorption spectra, J. Opt. Soc. Am. 58:192.

11. Scott, N.A. (1974) A direct method of computation of the transmission function of an inhomogeneous gaseous medium, I: Description of the method, J. Quant. Spect. Rad. Trans. 14:691.

12. Kunde, V.G., and McGuire, W.C. (1974) Direct integration transmittance model, J. Quant. Spect. Rad. Trans. 14:803.

Brigham[13] and Bracewell.[14] The sampling theorem states that if the Fourier transform of a function is zero for all frequencies greater than frequency f_o, then the continuous function g(x) can be uniquely determined from its sampled values, $g_s(n\delta x)$, if the sampling interval is chosen as

$$\delta x = \frac{1}{2f_o} \quad . \tag{19}$$

In particular, the continuous function g(x) can be reconstructed for all x by convolving the continuous interpolating function

$$s(x) = \frac{1}{\delta x} \frac{\sin\left(\pi \frac{x}{\delta x}\right)}{\left(\pi \frac{x}{\delta x}\right)} \tag{20}$$

with the sampled function $g_s(n\delta x)$ where n is integer. That is,

$$g(x) = g_s(n\delta x) * s(x) \tag{21}$$

or explicitly for the discrete convolution we have

$$g(x) = \sum_{n=-\infty}^{\infty} g_s(n\delta x) \frac{\sin \pi\left(\frac{x}{\delta x} - n\right)}{\pi\left(\frac{x}{\delta x} - n\right)} \, . \tag{22}$$

In the present case, the Fourier transform of the Lorentz function does not have a frequency, f_o, beyond which the transform is zero. Consequently by sampling at discrete intervals, it is not possible to exactly reconstruct the continuous function. However, by properly choosing the interval, the difference between the exact and reconstructed functions can be held within a predetermined limit. The Lorentz function is given as

$$g(x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + x^2} \tag{23}$$

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13. Brigham, E.O. (1974) The Fast Fourier Transform, Englewood Cliffs, New Jersey.

14. Bracewell, R.M. (1965) The Fourier Transform and Its Applications, McGraw-Hill, New York.

where $x = \nu - \nu_0$, α is the halfwidth, and ν_0 is the wavenumber value of the transition. The Fourier transform of $g(x)$ is

$$\mathcal{F}(g(x)) = \mathfrak{g}(f) = e^{-2\pi\alpha f} \tag{24}$$

where $\mathcal{F}$ is the Fourier transform operator. If the value of the transform is assumed to be zero beyond a frequency, f_0, this is equivalent to multiplying the complete transform by a rectangular box, $\mathscr{L}(f)$, where

$$\mathscr{L}(f) = \begin{cases} 1 & |f| < f_0 \\ \frac{1}{2} & |f| = f_0 \\ 0 & |f| > f_0 \end{cases} \tag{25}$$

We may define the sampling interval as before such that

$$\delta x = \frac{1}{2f_0} . \tag{26}$$

The Fourier transform of $\mathscr{L}(f)$ in the x domain is given by

$$s(x) = \frac{1}{\delta x} \frac{\sin\left(\pi \frac{x}{\delta x}\right)}{\left(\pi \frac{x}{\delta x}\right)} \tag{27}$$

which is identical to the scanning function prescribed by the Nyquist sampling theorem (Eq. (20)).

In order to evaluate the error caused by the discrete sampling interval and the associated truncation of the function in the Fourier domain, calculations have been made using the interpolating function, Eq. (27), convolved with the sampled Lorentz function

$$g_s(n\delta x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + (n\delta x)^2} \tag{28}$$

as indicated in Eq. (22). For these convolution calculations, a more relevant definition of the sampling interval, δx, is given in terms of the halfwidth, α,

$$\delta x = \frac{\alpha}{N} . \tag{29}$$

The results are evaluated for sampling intervals expressed in fractions, $1/N$, of the halfwidth. For this definition, we have for the sampled Lorentz function

$$g_s\left(\alpha \frac{n}{N}\right) = \frac{1}{\pi\alpha} \frac{1}{1+\left(\frac{n}{N}\right)^2} . \tag{30}$$

A quantitative evaluation of the effect of the sampling interval, is the RMS deviation of the function interpolated at three intermediate points per interval from the function calculated exactly at the same intermediate points. The results of these calculations are given in Table 2. These results are a measure of the amount of information lost due to the choice of sampling interval. As the sampling interval becomes infinitesimally small, the RMS deviation approaches zero. It is seen that for an interval of $\alpha/4$, that is, $N = 4$, the RMS deviation is negligibly small and essentially all of the information is retained.

Table 2. Effect of Sampling Interval on the Reconstruction of the Lorentz Function Using (sin x/x) Interpolation and Four Point Lagrange Interpolation. Interpolations are calculated at three equally spaced points between the sampled values. In all cases the maximum percent deviation using the four point Lagrange occurs in the first sampled interval. Deviations are calculated as the difference between the interpolated value and the exact value of the function

Sampling Interval		Interpolation Method		
		$\frac{\sin x}{x}$	Four Point Lagrange	
N	$\delta x = \frac{\alpha}{N}$	rms deviation	rms deviation	max percent deviation
1	α	1.1×10^{-3}	3.5×10^{-3}	-1.9
2	$\frac{\alpha}{2}$	0.067	0.20	-0.99
3	$\frac{\alpha}{3}$	0.0035	0.067	-0.37
4	$\frac{\alpha}{4}$	0.00063	0.026	-0.15

There is another consideration that must be taken into account in this situation. Although the information is retained for a sampling interval of $\alpha/4$, the computational effort to retrieve this information using the (sin x/x) interpolation is large and in some cases may be of the same magnitude as that required to evaluate the function directly at the intermediate intervals.

In order to retrieve sufficient information with reasonable computational effort and stay within a specified error criterion for the absorption coefficient calculation, a four point interpolation function has been used instead of the prohibitively long "sin x/x" interpolation. The output points are assumed to be equally spaced. Values for the weighting factors necessary to perform the interpolation at three equally spaced intermediate points are given by the following three equations:

$$g\left(x + \frac{\delta x}{4}\right) = -\frac{7}{128}\, g(x - \delta x) + \frac{105}{128}\, g(x) + \frac{35}{128}\, g(x + \delta x) - \frac{5}{128}\, g(x + 2\delta x) \tag{31}$$

$$g\left(x + \frac{\delta x}{2}\right) = -\frac{1}{16}\, g(x - \delta x) + \frac{9}{16}\, g(x) + \frac{9}{16}\, g(x + \delta x) - \frac{1}{16}\, g(x + 2\delta x) \tag{32}$$

$$g\left(x + \frac{3\delta x}{4}\right) = -\frac{5}{128}\, g(x - \delta x) + \frac{35}{128}\, g(x) + \frac{105}{128}\, g(x + \delta x) - \frac{7}{128}\, g(x + 2\delta x) \quad . \tag{33}$$

The interpolation scheme that has been employed in this development is due to Lagrange and is well described by Acton.[15] In Table 2, the maximum percent deviation in the interpolated values is indicated. This error always occurs within one or two intervals from the line center. For a sampling interval of $\alpha/4$, the error is 0.15 percent. Although this error at the line center is slightly larger than desirable, the added complication of using a more refined interpolation does not presently seem warranted. Furthermore, the percent error decreases rapidly away from the line center.

The four point interpolation scheme is used for interpolating the "very slow array," and the "slow array" into the "fast array." This is required since the sampling criterion of $\alpha/4$ has been used for the calculation of the three arrays where the effective α is appropriate to each array.

Similarly, for the presentation of the final results, the fast array is interpolated into a plotting array in a separate program which represents the final result. Figure 3 depicts the effect of this interpolation scheme as compared to the result obtained with linear interpolation. It should be noted that the error for a complete spectrum can only be the same or less than that for a single line. This is readily concluded from the superposition theorem.

One final consideration that provides information on the sampling interval, is the Rayleigh criterion.[16] For two spectral lines of unit strength and equal halfwidths, separated by two halfwidths, let us determine the sampling interval required to exactly reproduce the minimum between the two spectral lines.

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15. Acton, F. S. (1970) Numerical Methods That Work, New York.
16. Born, M., and Wolf, E. (1965) Principles of Optics, Oxford, Pergamon Press.

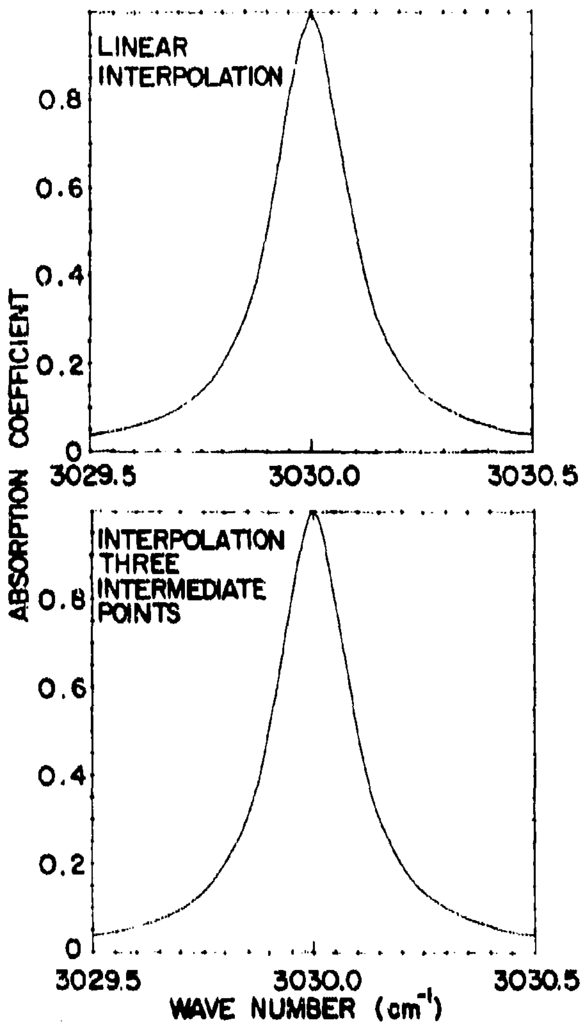

Figure 3. Reconstruction of the Shape of a Single Line of Strength π, halfwidth, $\alpha = 0.1$, Using a Sampling Interval of $\delta x = \alpha/4$ With a Sampling Point Positioned at the Spectral Line Center. The upper curve uses linear interpolation of the convolution output and the lower curve uses the 4 point Lagrange interpolation. To emphasize the line center, the region from -5 to +5 halfwidths is depicted

Consider one line centered at $x = 0$ and the other line centered at $x = x_o$. We have for the two Lorentz functions

$$g_1(x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + x^2} \tag{34}$$

and

$$g_2(x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + (x - x_o)^2} \quad . \tag{35}$$

The Fourier transform for this pair is given by

$$\mathcal{F}(f) = e^{-2\pi\alpha f} + e^{-2\pi\alpha f} \cos (2\pi x_o f) \quad . \tag{36}$$

The Rayleigh criterion postulates $x_o = 2\alpha$ giving for the transform

$$\mathcal{F}(f) = e^{-2\pi\alpha f} (1 + \cos 4\pi\alpha f) \quad . \tag{37}$$

To exactly reproduce the minimum between the doublet, one period of the oscillatory function is required, giving

$$4\pi\alpha f_o = 2\pi \tag{38}$$

so that the cut off frequency is

$$f_o = \frac{1}{2\alpha} \tag{39}$$

and the sampling interval from the Nyquist theorem, is

$$\delta x = \frac{1}{2f_o} = \alpha \quad . \tag{40}$$

This result indicates that the sampling interval of $\alpha/4$, previously determined, is well within the Rayleigh criterion for resolving a Lorentzian doublet separated by two halfwidths.

4. APPLICATION OF THE ALGORITHM

In the previous sections, two basic steps for an improved computational procedure to perform the convolution of the Lorentz line shape with a set of absorption line data have been described: (1) the decomposition of the line shape into bounded domains, and (2) the criterion for determining the sampling interval. In this section we describe the application of the algorithm to obtain the absorption coefficient as a function of wavenumber for a set of spectral line data parameters that are appropriate for the specified values of temperature, pressure, and column density. Three separate convolutions utilizing the fast (XF), the slow (XS), and the very slow (XVS) functions are performed on the data set. The results of the three convolutions for a specific set of data are displayed in transmittance in Figure 4. For this case the average halfwidth is of the order of 0.04 cm^{-1} so that the sampling interval used is $\delta x = \alpha/4 = 0.01\ cm^{-1}$. Each convolution function is sampled at approximately 24 values corresponding to intervals of 0.01 cm^{-1} for the fast function, 0.04 cm^{-1} for the slow function, and 0.16 cm^{-1} for the very slow function. Seventy-two (72) points have been sampled to reproduce the Lorentzian from -48 to +48 halfwidths instead of 384 (4 X 96) which would be required if the function were sampled at equal intervals of $\alpha/4$ (0.01 cm^{-1}). Consequently, the algorithm as applied in this case provides a computational savings of a factor 5 1/3. The actual saving using an optimized version of the conventional method compared to the present method is a factor of 10. The additional factor of two is due to the use of tabulated rather than calculated functions and to reduced overhead time in setting up the inner convolution loop. The results of the two computational methods are given in Figure 5 and no differences are discernable. It should be noted that the lower spectrum of Figure 5 is equivalent to the product of the three functions presented in Figure 4, since the functions are all on a transmittance scale.

Some further consideration needs to be given to the method described here with respect to the theoretical computational gain. If the assumption is made that the line shape function can be decomposed into M functions, and that the sampling interval is the same for the first decomposed function as for the total Lorentz function, $\alpha/4$, then the gain, G, is

$$G = \frac{N_{tot}}{\sum_{m}^{M} N_m \left(\frac{\delta x_1}{\delta x_m}\right)} \quad . \tag{41}$$

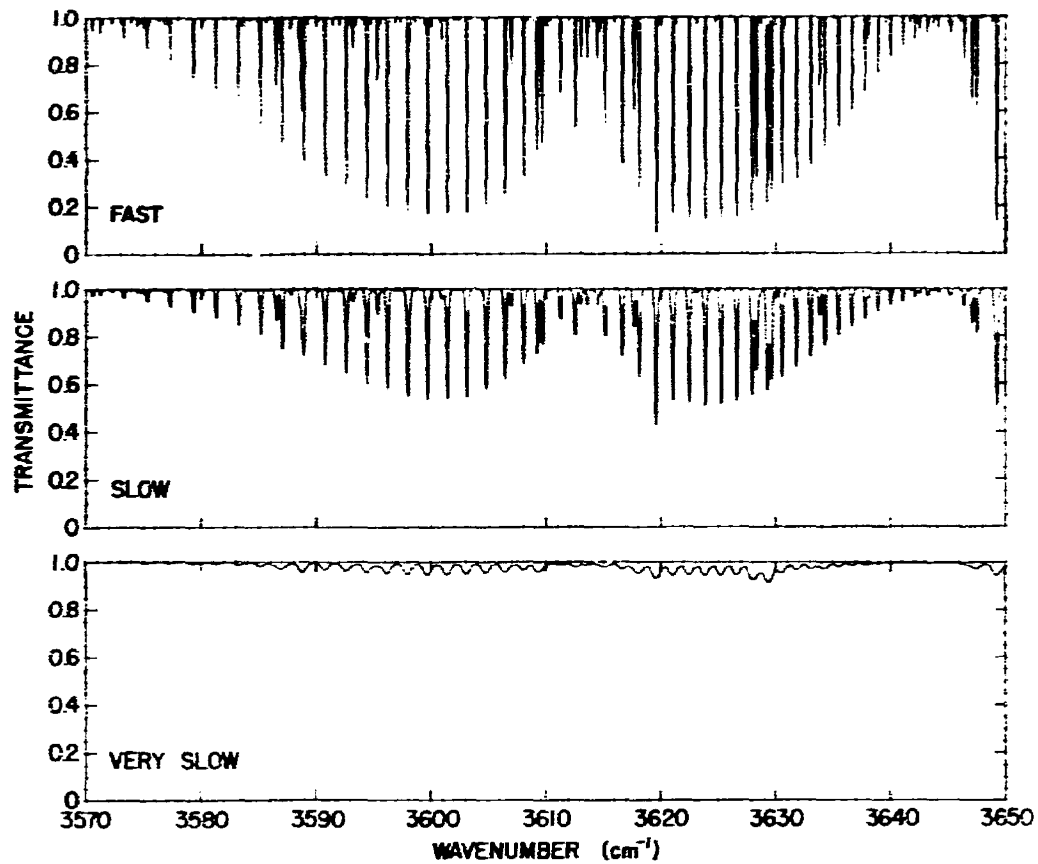

Figure 4. Results of the Convolution of the Three Individual Functions With the Spectral Line Data From 3570 cm^{-1} to 3650 cm^{-1} and a Sampling Interval DV = 0.01 cm^{-1}. From top to bottom the plots are the result of the fast function, slow function and very slow function convolutions respectively. The conditions are P = 500 millibars, T = 240 K, H_2O column density = $2.9 \times 10^{+18}$, and CO_2 column density = $7.6 \times 10^{+18}$ mol/cm^2. The results are expressed in transmission to increase the dynamic range of the presentation. The product of the three spectra give the total result shown in the upper spectrum of Figure 5

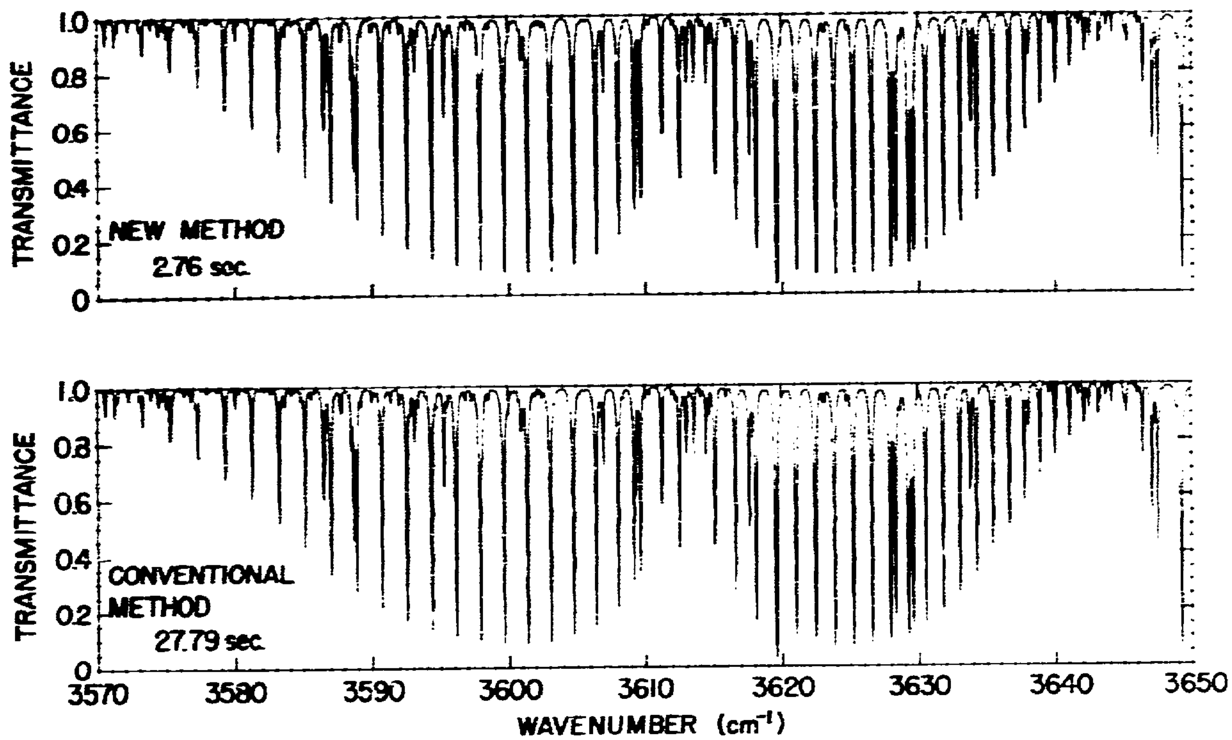

Figure 5. Spectral Transmission Results From 3570 cm^{-1} to 3650 cm^{-1} at a Sampling Interval of DV = 0.01 cm^{-1} for Conditions as in Figure 4: P = 500 millibars, T = 240 K, H_2O Column Density = $2.9 \times 10^{+18}$, and CO_2 Column Density = $7.6 \times 10^{+18}$ mol/cm^2. The upper trace is the result of the new algorithm and required 2.76 sec of computer time; the lower trace utilizing the conventional procedure required 27.79 sec. The times are for a CDC 6600 computer; read time has not been included. The AFGL line file was used for the spectral data from which 4401 lines were required

In this expression, N_{tot} is the total number of halfwidths over which the function is to be computed, N_m is the number of halfwidths spanned by the m'th decomposed function, and $\delta x_1/\delta x_m$ is the ratio of the sampling interval of the first function to that required for the m'th function. In the present case for $N_{tot} = 48$, we have:

$$G = \frac{48}{(3 \cdot 1 + 12 \cdot \frac{1}{4} + 48 \cdot \frac{1}{16})} = \frac{48}{9} = 5\frac{1}{3} \quad . \tag{42}$$

There are some constraints that are not explicit in the above expression; in particular, there are limitations on how small N_m can be and still have the function be reconstructable at the sampling interval. The algorithm provides greater improvement as the extent of the convolution is increased. For instance, if it were desired to reproduce the function over 192 halfwidths using four decomposed functions, a given choice would give a gain of

$$G = \frac{192}{(3 \cdot 1 + 12 \cdot \frac{1}{4} + 48 \cdot \frac{1}{16} + 192 \cdot \frac{1}{64})} = \frac{192}{12} = 16 \quad . \tag{43}$$

It must be emphasized that this choice, though workable, is not unique and other choices might provide greater improvement.

The algorithm, as it has been developed, must include protection against lines having halfwidths deviating significantly from the average. For anomalously wide lines, the convolution process can overflow the output arrays at the beginning and ending of the panels. In this case the line width is reset to the maximum width that can be treated: twice the average value. A series of + signs and the line identification are outputted when such a situation is encountered. In general, wide lines are not a problem since the widest lines do not vary significantly from the mean. This case also provides protection when a sampling interval, D[illegible] is chosen which is not consistent with the mean halfwidth of the lines being considered or when the line width is incorrect on the input data file.

There are a number of anomalously narrow lines that are encountered such as the high J, low K_a water lines of type measured by Eng et al.[17] For such lines, that is, $\alpha_i \ll \bar{\alpha}$, where α_i is the width of the i'th line and $\bar{\alpha}$ is the mean width, not only does the algorithm fail, but depending on the phasing of the sampling interval, the contribution of the transition can be missed entirely. Such lines have been

17. Eng, R.S., Kelley, P.L., Mooradian, A., Calawa, A.R., and Harmon, T.C. (1973) Tunable laser measurements of water vapor transitions in the vicinity of 5 μm, Chem. Phys. Letters 19:524.

treated by setting the halfwidth to the sampling interval, that is, α_i = DV. In this case, a series of – signs and the line identification are printed out. Although the convolution will be undersampled for such lines, information pertaining to the line is retained. The only strictly correct way to handle these narrow lines, is to choose a DV equal to $\alpha_i/4$ where α_i is characteristic of the narrowest line encountered. Such a choice of DV may necessitate the use of the conventional convolution method, since the sampling interval is so small. Computational requirements may dictate the calculation of the absorption coefficient over a small wavenumber region around the lines in question. In general, these lines are relatively weak, and except in cases such as laser transmission problems the method used here proves to be satisfactory.

5. EXTENSIONS OF THE METHOD

As has been indicated in the previous section, the calculation of the far line wings may be readily incorporated into the program. However, for the reasons stated it is recommended that this far wing contribution be handled as a continuum contribution in the wavenumber domain. Similarly, the variation of line shape with molecular species may be incorporated into the algorithm. It is well known that the wings of air broadened CO_2 lines are "subLorentzian" and a very slow function specific to the CO_2 molecular species could be utilized in place of the Lorentz very slow function. However, there is no compelling evidence that the subLorentzian behavior occurs within 5 cm^{-1} of the line center at atmospheric pressure so again, it is considered more appropriate to include the absorption due to the far wings of the CO_2 lines as a properly chosen continuum function. The best available theories indicate that the subLorentzian behavior is wavenumber dependent. Incorporation of this effect is not amenable to a direct extension of the algorithm since the argument of the Lorentz function is in terms of halfwidths. The wing modification may be readily added to the calculation by including the contribution into the very slow array before the three arrays are combined into the final output array. Continuum contributions of this type are important for CO_2 in spectral regions such as the 01001 band center where the wing contribution from the Q branch is not negligible as at 667.2 cm^{-1} and beyond the band head from 780 cm^{-1} to 890 cm^{-1}.

The convolution method described here offers even more significant computational savings for the multilayer case as it is generally applied to atmospheric modeling. The sampling interval is determined for each layer based on the average halfwidth which is a function of temperature and pressure for the layer. The remaining problem is to merge the results of each layer using appropriate

interpolation techniques to obtain the transmission or emission for the case being considered. In the conventional approach to the problem, the calculations are performed at the finest sampling interval required and is the same for all layers; that is, the sampling interval required to perform the absorption coefficient calculation at 60 km is the same as that used at 0 km. This approach requires the calculation of many more output points than is necessary at altitudes below the original altitude with a proportional increase in computational effort. With the scheme proposed here, the computational time is the same for each layer.

6. LINE SHAPES OTHER THAN LORENTZIAN

The present method is clearly not restricted to any particular function such as the Lorentz function. The Doppler line shape may readily be tabulated either directly or as decomposed functions depending on the definition of halfwidth. For many atmospheric modeling cases, the line shape of greatest interest is the Voigt[18] shape. Current efforts are being directed toward incorporating the Voigt line shape into the new algorithm. Preliminary indications are that the Voigt profile, computed to an accuracy similar to that attained for the Lorentz, will require only slightly more computer time than that required for the Lorentz function. Details of the procedure for calculating the Voigt shape will appear in a subsequent publication. Although the program assumes a symmetric line shape and only half the scanning function is stored, an asymmetric shape can be utilized by storing the entire function and making minor changes to the program.

7. THE PROGRAM

The program has been written to use line parameter input data consistent with that contained on the AFGL line parameter tape.[1] The line data is reformatted onto a binary file which contains the line data pertinent to the molecules and wavenumber range of interest. This step has been taken to keep read time consistent with the time required to perform the calculational part of the program. The control parameters are read from the input file and written to the output file; "tape 3" is the binary file containing the line parameter data; and KKFILE is the binary output file. KKFILE contains a header record which includes the identification information, SECANT, temperature, pressure, molecular identification, and molecular column densities of the homogeneous layer. The first record for each output panel is a header record for the panel which contains the wavenumber values

18. Voigt, S. Münch, Ber. (1912) p. 603.

of the first and last absorption coefficient values of the panel, the wavenumber increment between output points and the number of output points. The second record of the panel contains the array of absorption coefficient values resulting from the convolution calculation. The current version of the program outputs a maximum of 2400 values; in general, the first and last panel are shorter.

The program consists of the main program HIRACC; subroutines SHAPE, MOLEC, RDFILE, CONVFN, and PANEL; and the function QVRFAC. The overall strategy of the program is indicated in Figure 6. All the subroutines are called from the main program and the flow of the program is easily traced. Subroutine SHAPE sets up the three convolution functions XF, XS, XVS used to define the Lorentz function from 0 to 48 halfwidths.

Subroutine MOLEC in conjunction with function QVRFAC, makes the molecular identifications with the line parameter file, and determines the correction factors for the line intensities (SCOR) and the halfwidths (ALFCOR). The quantity, SCOR, is the correction factor due to the temperature dependence of the vibrational and rotational partition sums. The vibrational partition sum is calculated for a given molecular type as

$$Q_v(T) = \prod_{i=1}^{N} \frac{1}{\left(1 - e^{-h\nu_i/kT}\right)^{d_i}} \tag{44}$$

where ν_i is a fundamental vibrational frequency and d_i is the degeneracy of the vibration. The temperature dependence of the rotational partition sum is given by

$$\frac{Q_R(T_o)}{Q_R(T)} = \left(\frac{T_o}{T}\right)^F \tag{45}$$

where F = 1 for linear molecules and 1.5 for nonlinear molecules. The reference temperature, T_o, is taken as 296 K, consistent with the AFGL Line Listing. For further discussion of these topics, see Herzberg[19] pp 503 ff. The partition sum calculations are performed by QVRFAC and the necessary molecular parameters are contained in data statements in subroutine MOLEC. The quantity, ALFCOR, is the correction factor due to the pressure and temperature dependence of the collision broadened halfwidth. The temperature dependence of the halfwidth has

---

19. Herzberg, G. (1945) Molecular Spectra and Molecular Structure II. Infrared and Raman Spectra, D. Van Nostrand and Co., Princeton.

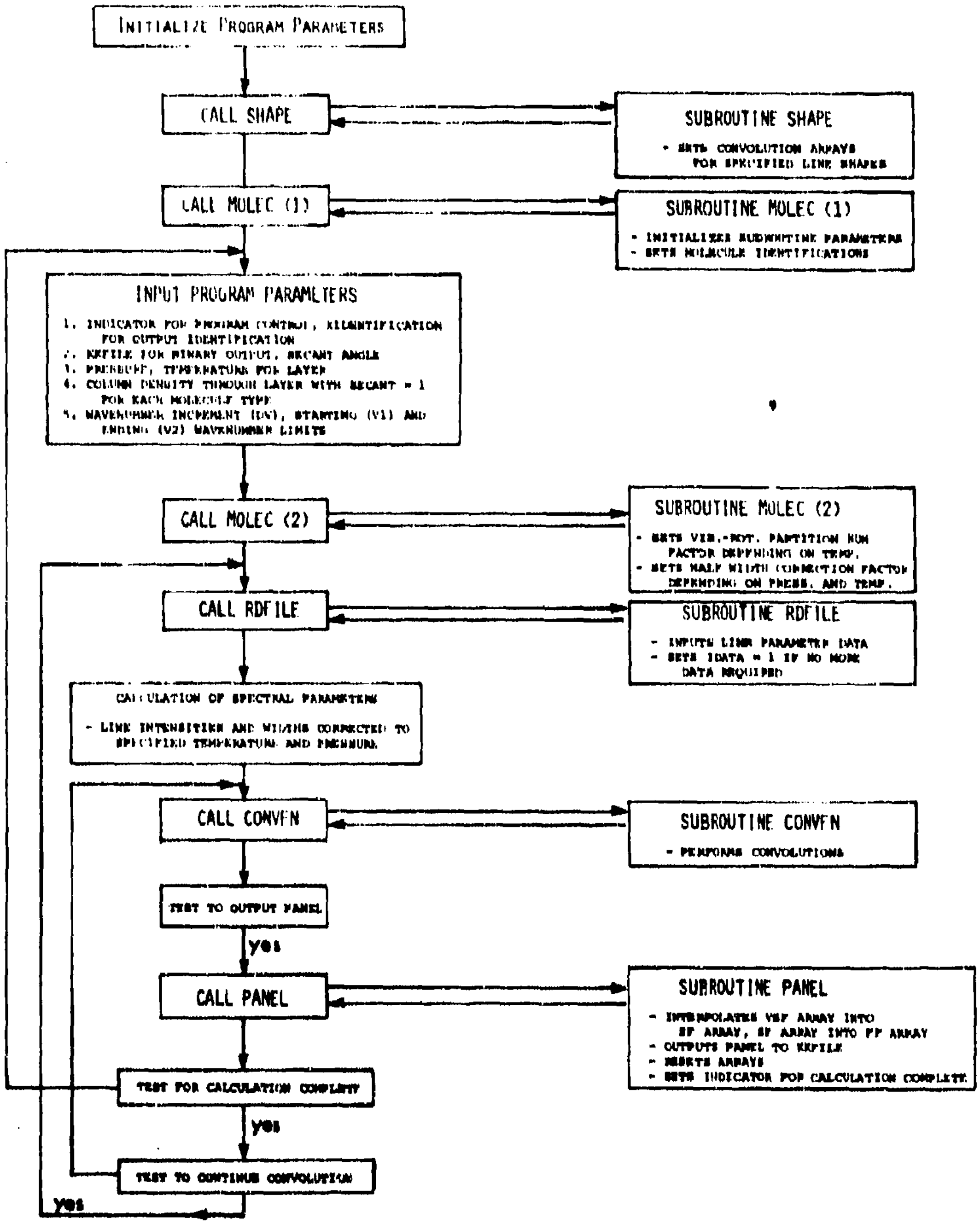

Figure 6. Flow Diagram for HIRACC Program

been taken as $(T_o/T)^{0.5}$ although calculations based on the Anderson - Tsao - Curnutte theory are reported to give a temperature dependence ≈ $(T_o/T)^{0.75}$ (Varanasi[20]).

Subroutine RDFILE reads the blocked binary line parameters over the wave-number range for which line data is required. The line parameters include the wavenumber value of the transition (GNU, cm^{-1}), the intensity of the transition at 296°K (S, $cm^{-1}/(mol/cm^2)$), the collision broadened halfwidth at half maximum for 296°K and atm pressure (ALFAO, cm^{-1}), the lower state energy of the transition (EPP, cm^{-1}), and the molecule identification number (MOL). If the line parameter data is insufficient to complete the specified calculation, the message "end of file on disk" is printed on the output file. If no further line data is required IDATA is set to 1, and control is returned to the main program.

At this stage of the main program, an effective optical depth is calculated for each line which is dependent on the column density of the layer, the secant of the angle through the layer, the temperature of the layer, and the halfwidth of the line, α(ALFI).

The effective depth, u',

$$u' = \left(\frac{1}{\alpha}\right) \cdot w \cdot \sec \cdot \left(\frac{Q_{VR}(T_o)}{Q_{VR}(T)}\right) \cdot \left[\exp\left(\frac{E''}{kT_o} - \frac{E''}{kT}\right)\right] \cdot \left[\frac{1 - \exp\left(-\frac{h\nu}{kT}\right)}{1 - \exp\left(-\frac{h\nu}{kT_o}\right)}\right] \tag{46}$$

where w is the absorber column density, E'' is the lower state energy, $Q_{VR} = Q_V Q_R$, and the other quantities have been previously defined. In terms of the program coding the effective depth appears as:

```
EFDPTH=RECALF*W*SEC*SCOR*EXP(EPP/XKTFAC)*(1.-EXP(-GNU/TEMPO))/
  (1.-EXP(-GNU/TAVE)).
```

As previously discussed, the proper sampling interval, DV, should be 0.25 times the average line halfwidth. If the halfwidth, ALFI, is less than the sampling interval, the halfwidth is set to the sampling interval and a series of minus signs is written to the output file. If the halfwidth exceeds a maximum value (ALFMAX) where ALFMAX = BOUND/48 and BOUND is the maximum value in wavenumbers over which a line can be calculated, the halfwidth is reset to ALFMAX, and a series of + signs is written to the output file. Included in the records indicating the

20. Varanasi, P., and Ko, F.K. (1977) Intensity and transmission measurements in the ν_3 fundamental of N_2O at low temperatures, Thirty Second Symposium on Molecular Spectroscopy, Paper RF'5, Columbus, Ohio

resetting of the halfwidth is the wavenumber value of the transition (GNU), the intensity (S) and the halfwidth (ALFAO) values of the transition from the line parameter tape, the calculated value of the halfwidth (ALFI), the value to which the halfwidth (DV or ALFMAX), and molecular identification number (M). If the number of halfwidth changes (NCHNG) exceeds 100, the computation is terminated.

Subroutine CONVFN is a tightly written subprogram in which considerable effort has been taken to minimize operations in the DO 30 loop. This subroutine performs the triple convolution of XF, XS, and XVS with the line data putting the results in the proper elements of FF, SF, and VSF respectively. A simplified flow diagram appears in Figure 7. Control indicator IPANEL is set to IDATA if the DO loop over the lines (40) is satisfied indicating whether a panel is complete or more lines are required. If the line DO loop (40) is not completed, IPANEL is set to 1 indicating that a complete panel has been calculated. Control is returned to the main program.

If IPANEL has been set to 1, subroutine PANEL is called. Subroutine PANEL performs a four point Lagrange interpolation of the VSF array into the SF array and the SF array into the FF array, thus combining the results of three independent convolutions into a final result. A general flow diagram of panel is given in Figure 8. Care is taken to store array values required for the interpolation of subsequent panels. VFT is the wavenumber value of the first element of the FF array, which is common to the first element of the SF and VSF arrays. A binary header record is written to the binary file (KKFILE) for each panel which includes the wavenumber value (V1P) of the first element of the panel (FF(NLO)), the wavenumber value (V2P) of the last element of the panel (FF(NHI)), the wavenumber increment (DV), and the number of absorption coefficient values outputted (NLIM). The second binary record contains the NLIM values of the absorption coefficient from the FF array. The arrays are appropriately shifted and reset in preparation for the computation of subsequent panels. Control is again returned to the main program, HIRACC.

After a panel is written to KKFILE, a record is written to the output file indicating the current value of the time, the time spent in RDFILE, in CONVFN, and in PANEL (the units are seconds). Also included in this record are the first and last wavenumber values of the panel, the wavenumber increment, and the number of values in the panel. A second record is written to the output file indicating the average value of the halfwidth, the number of lines read since the last panel was completed, and the total number of lines read since the initiation of the convolution calculation. Control is returned to statement 10 if the calculation is complete, or to statement 140 to continue the convolution process.

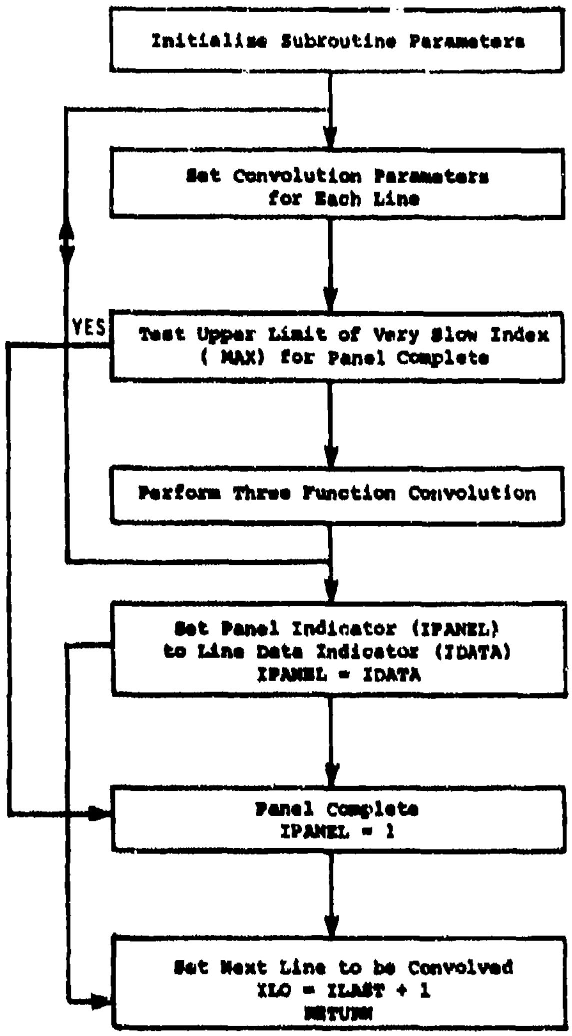

Figure 7. Flow Diagram for SUBROUTINE CONVFN

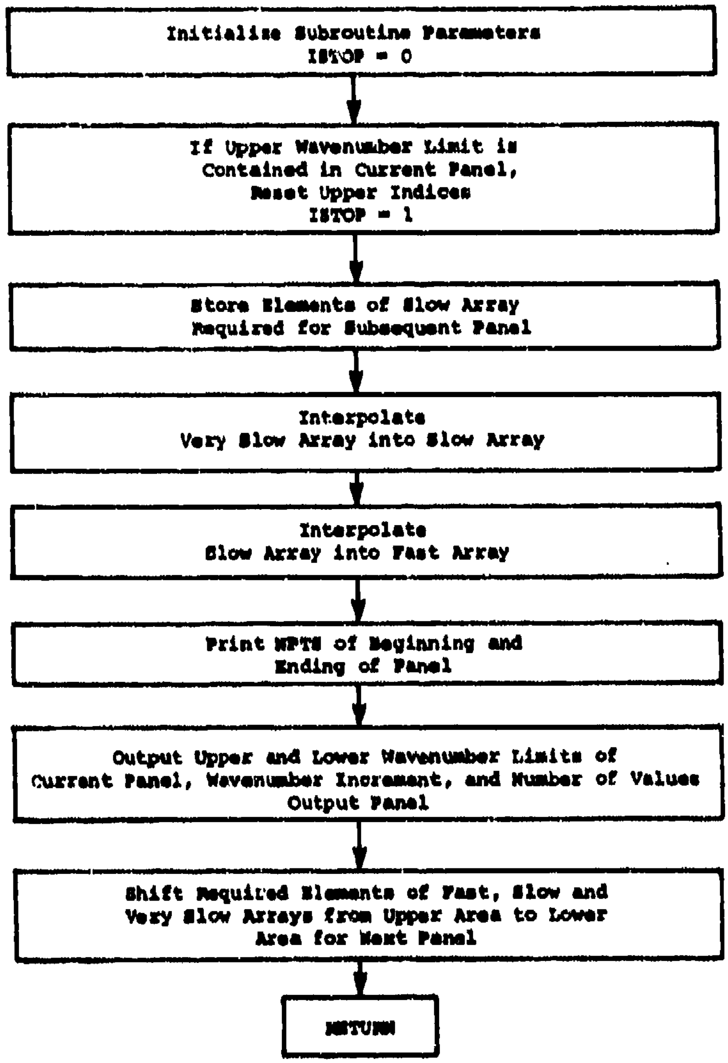

Figure 8. Flow Diagram for SUBROUTINE PANEL

References

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18. Voigt, S., and Münch, Ber. (1912) p. 603.

19. Herzberg, G. (1945) Molecular Spectra and Molecular Structure II. Infrared and Raman Spectra, D. Van Nostrand and Co., Princeton.

20. Varanasi, P., and Ko, F.K. (1977) Intensity and transmission measurements in the ν_3 fundamental of N_2O at low temperatures, Thirty Second Symposium on Molecular Spectroscopy, Paper RF'5, Columbus, Ohio.

Appendix A

A listing of the Fortran program HIRACC is given in Table A1, together with the loader map, the input data, and the program output for the results which appear in Figure 5. In the output, it should be noted that one line is encountered that has a halfwidth which is larger than that allowed by the program. This line at 3558.4830 cm^{-1} is an HDO line, molecular type 1, which has an erroneous halfwidth on the AFGL line tape used. The width for this line is reset to ALFMAX = 0.08 cm^{-1}. Two H_2O lines occur at 3579.0810 cm^{-1} which have anomalously narrow halfwidths. The values of these halfwidths are correct and are the high J, low K_A water lines of the type measured by Eng et al.[1] The widths for these lines are reset to DV = 0.01 cm^{-1}. The beginning and ending sections of the output panels are printed out including the location in the FF array, the dimensionless absorption coefficient, and the wavenumber value associated with the respective elements of the FF array.

1. Eng, R.S., Kelley, P.L., Mooradian, A., Calawa, A.R., and Harmon, T.C. (1973) Tunable laser measurements of water vapor transitions in the vicinity of 5 μm, Chem. Phys. Letters 19:524.

Table A1. Listing of HIRACC Program

```
      F4/74    OPT=1                                FTN 4.5+414        07/11/77

      PROGRAM HIRACC(INPUT,OUTPUT,TAPE3,TAPE10)
C
C
**********************************************************************
*                                                                    *
*                                                                    *
*             HIGH RESOLUTION ABSORPTION COEFFICIENT CODE            *
*                                                                    *
*                                                                    *
*     AUTHORS=  S. A. CLOUGH, F. X. KNEIZYS, AND J. H. CHETWYND      *
*                                                                    *
*                                                                    *
*           AIR FORCE GEOPHYSICS LABORATORY   (OPI)                  *
*           BEDFORD, MA   01731                                      *
*                                                                    *
*                                                                    *
*                                     DATE  JULY 11, 1977            *
*                                                                    *
*                                                                    *
**********************************************************************
*                                                                    *
*                                                                    *
*     CALCULATES MONOCHROMATIC ABSORPTION COEFFICIENT FOR SINGLE LAYER *
*                                                                    *
*     IND = INDICATOR TO CALCULATE (1) OR TO STOP (.NE.1)            *
*     XID= IDENTIFICATION (ALPHANUMERIC, SEVEN WORDS)                *
*     KKFILE = OUTPUT FILE NUMBER                                    *
*     SECANT = VALUE OF SECANT THROUGH LAYER                         *
*     PAVE = AVERAGE PRESSURE OF LAYER IN MILLIBARS                  *
*     TAVE = AVERAGE TEMPERATURE OF LAYER IN DEGREES KELVIN          *
*     W(M) = COLUMN DENSITY OF M'TH MOLECULE (FOR SECANT =1. )       *
*     DV SHOULD BE OF THE ORDER OF 0.25 OF THE AVERAGE HALF WIDTH    *
*     DV= OUTPUT INTERVAL IN WAVENUMBERS                             *
*     V1 = INITIAL WAVENUMBER VALUE TO BE COMPUTED                   *
*     V2 = FINAL WAVENUMBER VALUE TO BE COMPUTED                     *
*                                                                    *
*                                                                    *
**********************************************************************
C
C
      COMMON KK,KKFILE,PAVE,TAVE,U(7)
      COMMON GNU(250),S(250),ALFA0(250),EPP(250),MOL(250)
      COMMON FF(3200),SF(800),VSF(200)
      COMMON /XSUB/ RECPI,LIMIN,ILO,IHI,VBOT,VTOP,V1,V2,DV,VFT,IEOF,IPAN
     1EL,IDATA,ISTOP
      COMMON /NXX/ NWF,DXF,NF,NWS,DXS,NS,NWVS,DXVS,NXVS,NFMAX,NSMAX,NVSM
     1AX
      COMMON /SUB1/ MAXF,MAXS,MAXVS,NLIMF,NLIMS,NLIMVS,NLO,NHI,DVS,DVVS
      COMMON /XPANEL/ V1P,V2P,NLIM,NSHIFT,NPTS
      COMMON /XTIME/ TIME,TIMRDF,TIMCNV,TIMPNL
      DIMENSION XID(8),HMOLID(7),W(7),SCOR(7),ALFCOR(7)
      DIMENSION XF(201), XS(201), XVS(201)
      DIMENSION EPDPTH(1), RECALF(1)
      EQUIVALENCE (S,EPDPTH), (ALFA0,RECALF)
      PI=2.*ASIN(1.)
      RECPI=1./PI
      NPTS=10
      NWF=3
      DXF=0.02
      NF=151
      NWS=12
      DXS=0.08
      NS=151
      NWVS=48
      DXVS=.32
      NXVS=151
      NFMAX=201
      NSMAX=201
      NVSMAX=201
      NSHIFT=32
      NLIMF=2400+1
      NLIMS=(NLIMF/4)+1
      NLIMVS=(NLIMS/4)+1
C     NOTE (DXVS/DXF) IS 16 AND (DXVS/DXS) IS 4
```

Table A 1. Listing of HIRACC Program (Cont.)

```
PROGRAM HIRACC
              NBOUND=48.*(DXVS/DXF)
              MAXF=NLIMF+NBOUND
              MAXS=(MAXF/4)+1
              MAXVS=(MAXS/4)+1
              CALL SHAPE (XF,YS,XVS)
              CALL MOLEC(1,MMOLID,7,TEMPO,TAVE,PO,PAVE,SCOR,ALFCOR)
              LININ=250
       10     PRINT 900
              TIMROF=TIMONV=TIMPNL=0.
              READ 902, IND,(XID(I),I=1,7)
              IF (IND.NE.1) GO TO 160
              PRINT 904,    (XID(I),I=1,7)
              REWIND 3
              IEOF=0
              READ 905, KKFILE,SECANT
              PRINT 910, KKFILE
              PRINT 915, SECANT
              READ 920, PAVE,TAVE
              PRINT 925, PAVE,TAVE
              READ 920, (W(M),M=1,7)
              PRINT 930, (MMOLID(M),W(M),M=1,7)
              READ 935, DV,V1,V2
              PRINT 940, DV,V1,V2
              IF (DV.LE.0.0) GO TO 160
              DVS=(DXS/DXF)*DV
              DVVS=(DXVS/DXF)*DV
              BOUND=FLOAT(NBOUND)*DV/2.
              PRINT 942, BOUND
              ALFMAX=BOUND/48.
              NLO=NBOUND+1
              NHI=NLIMF+NSHIFT-1
              DO 50 I=1,MAXF
       50     FF(I)=0.
              DO 60 I=1,MAXS
       60     SF(I)=0.
              DO 70 I=1,MAXVS
       70     VSF(I)=0.
              PRINT 900
       C
              WRITE (KKFILE) (XID(I),I=1,7),SECANT,PAVE,TAVE,(MMOLID(M),M=1,7),
             1  (W(M),M=1,7),   DV,V1,V2
       C
              VFT=V1-2.*BOUND
              VBOT=V1-BOUND
              VTOP=V2+BOUND
       C
              P0=1013.0
              TEMP0=296.0
              XKT0=0.6951*TEMP0
              XKT =0.6951*TAVE
              XKTFAC= (1./XKT0) - (1./XKT)
              CALL MOLEC(2,MMOLID,7,TEMPO,TAVE,P0,PAVE,SCOR,ALFCOR)
              DO 80 M=1,7
       80     U(M)=W(M)*SCOR(M)*SECANT
              LIMCNT=0
              NCHNG=0
       C
       90     CONTINUE
              ICNT=0
              SUMALF=0.
       C
       100    CONTINUE
       C
              CALL SECOND (TIME0)
              IF (IEOF.NE.0) GO TO 150
              CALL RDFILE (GNU,S,ALFA0,EPP,MOL)
              CALL SECOND (TIME)
              TIMROF=TIMROF+TIME-TIME0
       C
              IF (IEOF.NE.0) GO TO 140
       C
       C      MODIFY LINE DATA FOR TEMPERATURE,PRESSURE, AND COLUMN DENSITY
       C
              DO 130 I=ILO,IHI
              M=MOL(I)
              EPOPTH(I)=S(I)*U(M)
```

Table A1. Listing of HIRACC Program (Cont.)

```
PROGRAM HIRACC
          IF (EFDPTH(I).LE.0.) GO TO 130
          ICNT=ICNT+1
          ALFI=ALFA0(I)*ALFOOR(M)
          IF (ALFI.GE.DV) GO TO 110
          PRINT 945, GNU(I),S(I),ALFA0(I),ALFI,DV,M
          ALFI=DV
          NCHNG=NCHNG+1
  110     IF (ALFI.LE.ALFMAX) GO TO 120
          PRINT 950, GNU(I),S(I),ALFA0(I),ALFI,ALFMAX,M
          ALFI=ALFMAX
          NCHNG=NCHNG+1
  120     CONTINUE
          SUMALF=SUMALF+ALFI
          RECALF(I)=1./ALFI
          EFDPTH(I)=EFDPTH(I)*EXP(EPP(I)*XKTFAC)*RECALF(I)*
         $    (1.-EXP(-GNU(I)/TAVE))/(1.-EXP(-GNU(I)/TEMP0))
  130     CONTINUE
          IF (NCHNG.GT.100) GO TO 160
  140     CONTINUE
C
          CALL CONVFN (GNU,EFDPTH,RECALF,MOL,FF,SF,VSF,XF,XS,XVS)
C
          IF (IPANEL.EQ.0) GO TO 100
C
  150     CONTINUE
C
          CALL PANEL (FF,SF,VSF,KKFILE)
C
          CALL SECOND (TIME)
          PRINT 955, TIME,TIMRDF,TIMCNV,TIMPNL,V1P,V2P,DV,NLIM
          AVALF=SUMALF/FLOAT(ICNT)
          LINCNT=LINCNT+ICNT
          PRINT 960, AVALF,ICNT,LINCNT
          SUMALF=0.
          ICNT=0
          IF (ISTOP.NE.1) GO TO 140
          END FILE KKFILE
          GO TO 10
C
  160     CONTINUE
          STOP
C
C
C
  900     FORMAT (1H1)
  902     FORMAT(I1,7A10)
  904     FORMAT(1X,7A10)
  905     FORMAT(I5,F15.6)
  910     FORMAT(*0 OUTPUT FILE NO. =* I5)
  915     FORMAT(*0 SECANT =* F15.5)
  920     FORMAT (10(1PE10.3))
  925     FORMAT(*0 PRESS(MB) =* F12.5/ *0 TEMP(K) =* F11.2)
  930     FORMAT(33H0 COLUMN DENSITY(MOLECULES/CM**2)   ,
         1  /   /(5X,A6, * = * 1PE10.3) )
  935     FORMAT (5F10.4)
  940     FORMAT(*0 DV(CM-1) = *F12.4/*0 V1(CM-1) = *F12.4/*0 V2(CM-1) = *
         1  F12.4)
  942     FORMAT(17H0 2*BOUND(CM-1) = ,F8.4)
  945     FORMAT (* ---------------------------*F10.4,E14.3,3F10.6,I5)
  950     FORMAT (* +++++++++++++++++++++++++++*F10.4,E14.3,3F10.6,I5)
  955     FORMAT (1H0,10X,*TIME*,11X,*READ*,4X,*CONVOLUTION*,10X,*PANEL*,8X,
         1*V1*,13X,*V2*,11X,*DV*8X,*NVALUES*,/4F15.3,2F15.4,F10.4,I10)
  960     FORMAT (*0  AVERAGE WIDTH = *F10.5,*     NO. LINES = *I10,
         1           *     TOTAL NO. OF LINES=*I10//)
          END
```

Table A1. Listing of HIRACC Program (Cont.)

```
SUBROUTINE SHAPE       74/74    OPT=1                                FTN 4.5+414        07/11/77

      SUBROUTINE SHAPE (XF,XS,XVS)
      COMMON /XSUM/ RECPI
      COMMON /NXX/ NWF,DXF,NF,NWS,DXS,NS,NWVS,DXVS,NXVS,NFMAX,NSMAX,NVSM
     1AX
      DIMENSION XF(1), XS(1), XVS(1)
      XLORNZ(X2)=1./(1.+X2)
      SFN(X2)=A1+B1*X2+C1*X2*X2
      VSFN(X2)=A2+B2*X2+C2*X2*X2
      A0(Z0)=(1.+3.*Z0**2+3.*Z0**4)/(1.+Z0**2)**3
      B0(Z0)=-(1.+3.*Z0**2)/(1.+Z0**2)**3
      C0(Z0)=1./(1.+Z0**2)**3
C     MATCH AT Z1 HALFWIDTHS
      Z1=4.
      A1=A0(Z1)
      B1=B0(Z1)
      C1=C0(Z1)
C     MATCH AT Z2 HALFWIDTHS
      Z2=12.
      A2=A0(Z2)
      B2=B0(Z2)
      C2=C0(Z2)
      TOTAL=0.
      DO 10 I=1,NFMAX
   10 XF(I)=0.
      XF(1)=RECPI*(XLORNZ(0.)-SFN(0.))
      SUM=XF(1)
      DO 20 JJ=2,NF
      X=FLOAT(JJ-1)*DXF
      X2=X*X
      XF(JJ)=RECPI*(XLORNZ(X2)-SFN(X2))
      SUM=SUM+XF(JJ)*2.
   20 CONTINUE
      XF(NF)=0.
      SUM=SUM*DXF
      TOTAL=TOTAL+SUM
      DO 30 I=1,NSMAX
   30 XS(I)=0.
      XS(1)=RECPI*(SFN(0.)-VSFN(0.))
      SUM=XS(1)
      NS1=FLOAT(NWF)/DXS+1.001
      DO 40 JJ=2,NS1
      X=FLOAT(JJ-1)*DXS
      X2=X*X
      XS(JJ)=RECPI*(SFN(X2)-VSFN(X2))
      SUM=SUM+XS(JJ)*2.
   40 CONTINUE
      NS1P=NS1+1
      DO 50 JJ=NS1P,NS
      X=FLOAT(JJ-1)*DXS
      X2=X*X
      XS(JJ)=RECPI*(XLORNZ(X2)-VSFN(X2))
      SUM=SUM+XS(JJ)*2.
   50 CONTINUE
      XS(NS)=0.
      SUM=SUM*DXS
      TOTAL=TOTAL+SUM
      DO 60 I=1,NVSMAX
   60 XVS(I)=0.
      XVS(1)=RECPI*VSFN(0.)
      SUM=XVS(1)
      NVS1=FLOAT(NWS)/DXVS+1.001
      DO 70 JJ=2,NVS1
      X=FLOAT(JJ-1)*DXVS
      X2=X*X
      XVS(JJ)=RECPI*VSFN(X2)
      SUM=SUM+XVS(JJ)*2.
   70 CONTINUE
      NS1P=NVS1+1
      DO 80 JJ=NS1P,NXVS
      X=FLOAT(JJ-1)*DXVS
      X2=X*X
      XVS(JJ)=RECPI*(XLORNZ(X2))
      SUM=SUM+XVS(JJ)*2.
   80 CONTINUE
      SUM=SUM*DXVS
      TOTAL=TOTAL+SUM
      RETURN
C
C
C
      END
```

Table A1. Listing of HIRACC Program (Cont.)

```
SUBROUTINE MOLEC      74/74    OPT=1                          FTN 4.5+414        07/11/77

      SUBROUTINE MOLEC(IND,HMOLID,NMOLEC,TEMP0,TEMP,P0,P,SCOR,ALFCOR)
      DIMENSION HMOLID(1),SCOR(1),ALFCOR(1)
      DIMENSION W(7,4),ND(7,4)
      COMMON /XMOLEC/ HM(7),NV(7),W1(7),N1(7),W2(7),N2(7),
     1  W3(7),N3(7),W4(7),N4(7),QV0(7),ROTFAC(7)
      DATA HM(1),NV(1),W1(1),N1(1),W2(1),N2(1),W3(1),N3(1),W4(1),N4(1),
     1              QV0(1),ROTFAC(1)/
     1 6H  H2O ,3, 3651.7,1, 1595.0,1, 3755.8,1,     0. ,0, 1.0004, 1.5 /
      DATA HM(2),NV(2),W1(2),N1(2),W2(2),N2(2),W3(2),N3(2),W4(2),N4(2),
     2              QV0(2),ROTFAC(2)/
     2 6H  CO2 ,3, 1364.0,1,  667.3,2, 2349.3,1,     0. ,0, 1.0040, 1.0 /
      DATA HM(3),NV(3),W1(3),N1(3),W2(3),N2(3),W3(3),N3(3),W4(3),N4(3),
     3              QV0(3),ROTFAC(3)/
     3 6H   O3 ,3, 1103.2,1,  700.9,1, 1042.1,1,     0. ,0, 1.0456, 1.5 /
      DATA HM(4),NV(4),W1(4),N1(4),W2(4),N2(4),W3(4),N3(4),W4(4),N4(4),
     4              QV0(4),ROTFAC(4)/
     4 6H  N2O ,3, 1284.9,1,  588.8,2, 2223.8,1,     0. ,0, 1.1267, 1.0 /
      DATA HM(5),NV(5),W1(5),N1(5),W2(5),N2(5),W3(5),N3(5),W4(5),N4(5),
     5              QV0(5),ROTFAC(5)/
     5 6H   CO ,1, 2143.3,1,      0. ,0,     0. ,0,     0. ,0, 1.0000, 1.0 /
      DATA HM(6),NV(6),W1(6),N1(6),W2(6),N2(6),W3(6),N3(6),W4(6),N4(6),
     6              QV0(6),ROTFAC(6)/
     6 6H  CH4 ,4, 2914. ,1, 1533.3,2, 3018.9,3, 1297.9,3, 1.0066, 1.5 /
      DATA HM(7),NV(7),W1(7),N1(7),W2(7),N2(7),W3(7),N3(7),W4(7),N4(7),
     7              QV0(7),ROTFAC(7)/
     7 6H   O2 ,1, 1403.5,1,     0. ,0,     0. ,0,     0. ,0, 1.0007, 1.0 /
C
C     MOLEC MAKES THE MOLECULAR IDENTIFICATIONS
C
C
C
C     ALFCOR IS THE FACTOR BY WHICH THE COLLISION WIDTH MUST BE CHANGED
C        DUE TO THE DEPENDENCE ON PRESSURE AND TEMPERATURE
C        THE TEMPERATURE DEPENDENCE IS TAKEN AS (T0/T)**0.5
C
C     SCOR IS THE FACTOR BY WHICH THE LINE INTENSITY IS CHANGED DUE TO
C        TEMPERATURE DEPENDENCE OF THE VIB AND ROT PARTITION SUMS
C
      IF (IND.EQ.2) GO TO 20
      MDIM=7
      NVDIM=4
      DO 10 M=1,NMOLEC
      W(M,1)=W1(M)
      W(M,2)=W2(M)
      W(M,3)=W3(M)
      W(M,4)=W4(M)
      ND(M,1)=N1(M)
      ND(M,2)=N2(M)
      ND(M,3)=N3(M)
      ND(M,4)=N4(M)
   10 HMOLID(M)=HM(M)
      RETURN
   20 CONTINUE
      PRATIO=P/P0
      TRATIO=TEMP0/TEMP
      DO 30 M=1,NMOLEC
      SCOR(M)=QVRFAC(M,TEMP,TRATIO,QV0,ROTFAC,W,ND,MDIM,NVDIM)
      ALFCOR(M)=PRATIO*(TRATIO**0.5)
   30 CONTINUE
      RETURN
      END
```

Table A 1. Listing of HIRACC Program (Cont.)

```
FUNCTION QVRFAC      74/74    OPT=1                          FTN 4.6+414         07/11/77

            FUNCTION QVRFAC(M,TEMP,TRATIO,QV0,ROTFAC,W,ND,MDIM,NVDIM)
            DIMENSION QV0(1),ROTFAC(1)
            DIMENSION W(MDIM,NVDIM),ND(MDIM,NVDIM)
            QV=1.
            DO 10 I=1,NVDIM
            IF (ND(M,I).EQ.0) GO TO 20
            SV=1.-EXP(-W(M,I)/TEMP)
            IF (ND(I).GT.1) SV=SV**ND(M,I)
    10      QV=QV/SV
    20      QVRFAC=(QV0(M)/QV)*((TRATIO)**ROTFAC(M))
            RETURN
    C
            END
```

```
SUBROUTINE RDFILE      74/74    OPT=1                        FTN 4.6+414         07/11/77

            SUBROUTINE RDFILE (GNU,S,ALFA0,EPP,MOL)
            COMMON /XSUB/ NEOPI,LIMIN,ILO,IHI,VBOT,VTOP,V1,V2,DV,VFI,IEOF,IPAN
           1EL,IDATA,ISTOP
            DIMENSION GNU(1), S(1), ALFA0(1), EPP(1), MOL(1)
            IDATA=0
    10      READ (3) VMIN,VMAX,NREC
            IF (EOF(3)) 90,20
    20      IF (VMAX.GE.VBOT) GO TO 30
            READ (3) VMIN
            GO TO 10
    30      READ (3) (GNU(I),S(I),ALFA0(I),EPP(I),MOL(I),I=1,NREC)
            ILO=1
            IHI=NREC
            IF (VMIN.GE.VBOT) GO TO 50
            DO 40 I=1,NREC
            ILO=I
            IF (GNU(I).GE.VBOT) GO TO 50
    40      CONTINUE
    50      IF (VMAX.LE.VTOP) RETURN
            DO 60 I=1,NREC
            IHI=I
            IF (GNU(I).GT.VTOP) GO TO 70
    60      CONTINUE
    70      IF (IHI.LT.NREC) IDATA=1
            RETURN
    90      PRINT 920
            IEOF=1
    100     RETURN
    C
    C
    920     FORMAT (* END OF FILE ON DISK*)
            END
```

Table A1. Listing of HIRACC Program (Cont.)

```
SUBROUTINE CONVFN     74/74    OPT=1                       FTN 4.5+414        07/11/77

               SUBROUTINE CONVFN (GNU,EFDPTH,RECALF,MOL,FF,SF,VSF,XF,XS,XVS)       004110
               COMMON /XSUB/ RECPI,LIMIN,ILO,IHI,VBOT,VTOP,V1,V2,DV,VFT,IEOF,IPAN  004120
              1EL,IDATA,ISTOP                                                      004130
               COMMON /XXX/ NWF,DXF,NF,NWS,DXS,NS,NWVS,DXVS,NXVS,NFMAX,NSMAX,NVSM  004140
              1AX                                                                  004150
               COMMON /SUB1/ MAXF,MAXS,MAXVS,NLIMF,NLIMS,NLIMVS,NLO,NHI,DVS,DVVS   004160
               COMMON /XTIME/ TIME,TIMRDF,TIMCNV,TIMPNL                            004170
               DIMENSION GNU(1), EFDPTH(1), RECALF(1), FF(1), SF(1)                004180
               DIMENSION MOL(1)                                                    004190
               DIMENSION XF(1), XS(1), XVS(1), VSF(1)                              004200
         C                                                                         004210
         C                                                                         004220
         C     THE VERY SLOW FUNCTION IS USED TO DRIVE THE CONVOLUTION PROCESS     004230
         C                                                                         004240
         C     THE VERY SLOW CONVOLUTION IS PERFORMED FROM -NWVS TO +NWVS IN       004250
         C     HALFWIDTHS                                                          004260
         C                                                                         004270
         C     DXVS IS THE INTERVAL AT WHICH THE VERY SLOW FUNCTION IS STORED IN   004280
         C     HALFWIDTHS                                                          004290
         C                                                                         004300
         C     JJ IS THE LOCATION IN THE VSF ARRAY FOR WHICH THE CONTRIBUTION      004310
         C     TO THE ABSORPTION COEFFICIENT FROM THE I'TH LINE IS CALCULATED      004320
         C                                                                         004330
         C     IZVS IS THE APPROPRIATE INDEX OF THE XVS FUNCTION                   004340
         C                                                                         004350
         C     VFT IS THE WAVENUMBER VALUE OF LOCATION 1 OF THE FF,SF AND VSF      004360
         C     ARRAYS                                                              004370
         C                                                                         004380
         C     DEPTHI= EFFECTIVE ABSORPTION COEFFICIENT OF THE I'TH LINE           004390
         C                                                                         004400
         C                                                                         004410
               CALL SECOND (TIMEO)                                                 004420
               RATVX=DVVS/DXVS                                                     004430
               FVS=FLOAT(NWVS)/DXVS                                                004440
               CONF=DVVS/DV-1.                                                     004450
               CONS=DVVS/DVS-1.                                                    004460
               IF (ILO.GT.IHI) GO TO 50                                            004470
               DO 40 I=ILO,IHI                                                     004480
               DEPTHI=EFDPTH(I)                                                    004490
               IF (DEPTHI.LE.0.) GO TO 40                                          004500
               ZSLOPE=RECALF(I)*RATVX                                              004510
               ZINT=(GNU(I)-VFT)/DVVS                                              004520
               RFVS=FVS/ZSLOPE                                                     004530
               JMAX=(ZINT+RFVS)+2.                                                 004540
               IF (JMAX.LE.MAXVS) GO TO 20                                         004550
               ILAST=I-1                                                           004560
               GO TO 55                                                            004570
            20 JMIN=(ZINT-RFVS)+2.                                                 004580
               JMINF=(ZINT*CONF)                                                   004590
               JMINS=(ZINT*CONS)                                                   004600
               ZVS=(FLOAT(JMIN-2)-ZINT)*ZSLOPE                                     004610
               ZS=ZVS+(FLOAT(JMINS)-ZINT*CONS)*ZSLOPE                              004620
               ZF=ZVS+(FLOAT(JMINF)-ZINT*CONF)*ZSLOPE                              004630
               DO 30 JJ=JMIN,JMAX                                                  004640
               JS=JMINS+JJ                                                         004650
               JF=JMINF+JJ                                                         004660
               ZVS=ZVS+ZSLOPE                                                      004670
               ZS=ZS+ZSLOPE                                                        004680
               ZF=ZF+ZSLOPE                                                        004690
               IZVS=ABS(ZVS)+1.5                                                   004700
               IZS=ABS(ZS)+1.5                                                     004710
               IZF=ABS(ZF)+1.5                                                     004720
               VSF(JJ)=VSF(JJ)+DEPTHI*XVS(IZVS)                                    004730
               SF(JS)=SF(JS)+DEPTHI*XS(IZS)                                        004740
               FF(JF)=FF(JF)+DEPTHI*XF(IZF)                                        004750
            30 CONTINUE                                                            004760
            40 CONTINUE                                                            004770
               ILAST=IHI                                                           004775
         C       IDATA=0 IF MORE DATA REQUIRED ** IDATA=1 IF NO MORE DATA REQUIRE  004780
               IPANEL=IDATA                                                        004790
               GO TO 60                                                            004800
            50 CONTINUE                                                            004810
               IPANEL=1                                                            004820
            60 ILO=ILAST+1                                                         004830
               CALL SECOND (TIME)                                                  004840
               TIMCNV=TIMCNV+TIME-TIMEO                                            004850
               RETURN                                                              004860
         C                                                                         004870
         C                                                                         004880
         C                                                                         004890
               END                                                                 004900
```

Table A1. Listing of HIRACC Program (Cont.)


```
      SUBROUTINE PANEL (FF,SF,VSF,KKFILE)
      COMMON /XSUB/ RECPI,LIMIN,ILO,IHI,VBOT,VTOP,V1,V2,DV,VFT,IFUF,IPAN
     1FL,IDATA,ISTOP
      COMMON /SUB1/ MAXF,MAXS,MAXVS,NLIMF,NLIMS,NLIMVS,NLO,NHI,DVS,DVVS
      COMMON /XPANEL/ V1P,V2P,NLIM,NSHIFT,NPTS
      COMMON /XTIME/ TIME,TIMRDF,TIMCNV,TIMPNL
      DIMENSION FF(1), SF(1), VSF(1)
      DIMENSION SFSTOR(8)
      CALL SECOND (TIME0)
      X00=-7./128.
      X01=105./128.
      X02=35./128.
      X03=-5./128.
      X10=-1./16.
      X11=9./16.
      ISTOP=0
      NNHI=(V2-VFT)/DV+1.5
      IF (NHI.GE.NNHI) ISTOP=1
      IF (ISTOP.EQ.1) NHI=NNHI
      JMXPR=NLO+NPTS
      JJPR=NHI-NPTS
      LIMLO=(NLO-1)/4-3
      LIMHI=(NHI/4)+1
C     SLOW FUNCTION VALUES NEEDED FOR SUBSEQUENT PANELS ARE SAVED
      DO 10 J=1,8
   10 SFSTOR(J)=SF(LIMHI+J-5)
      DO 20 J=LIMLO,LIMHI,4
      JVS=(J-1)/4+1
      SF(J)=SF(J)+VSF(JVS)
      SF(J+1)=SF(J+1)+X00*VSF(JVS-1)+X01*VSF(JVS)+X02*VSF(JVS+1)+X03*VSF
     1(JVS+2)
      SF(J+2)=SF(J+2)+X10*(VSF(JVS-1)+VSF(JVS+2))+X11*(VSF(JVS)+VSF(JVS+
     11))
      SF(J+3)=SF(J+3)+X03*VSF(JVS-1)+X02*VSF(JVS)+X01*VSF(JVS+1)+X00*VSF
     1(JVS+2)
   20 CONTINUE
      DO 30 J=NLO,NHI,4
      JS=(J-1)/4+1
      FF(J)=FF(J)+SF(JS)
      FF(J+1)=FF(J+1)+X00*SF(JS-1)+X01*SF(JS)+X02*SF(JS+1)+X03*SF(JS+2)
      FF(J+2)=FF(J+2)+X10*(SF(JS-1)+SF(JS+2))+X11*(SF(JS)+SF(JS+1))
      FF(J+3)=FF(J+3)+X03*SF(JS-1)+X02*SF(JS)+X01*SF(JS+1)+X00*SF(JS+2)
   30 CONTINUE
      IF (NPTS.EQ.0) GO TO 60
      DO 40 J=NLO,JMXPR
      VP=VFT+FLOAT(J-1)*DV
   40 PRINT 900, J,FF(J),VP
      DO 50 J=JJPR,NHI
      VP=VFT+FLOAT(J-1)*DV
   50 PRINT 900, J,FF(J),VP
   60 CONTINUE
      DO 70 J=1,8
   70 SF(LIMHI+J-5)=SFSTOR(J)
      NLIM=NHI-NLO+1
      V1P=VFT+FLOAT(NLO-1)*DV
      V2P=VFT+FLOAT(NHI-1)*DV
C     V1P IS FIRST FREQ OF PANEL
C     V2P IS LAST FREQ OF PANEL
      WRITE (KKFILE) V1P,V2P,DV,NLIM
      WRITE (KKFILE) (FF(J),J=NLO,NHI)
      VFT=VFT+FLOAT(NLIMF-1)*DV
      IF (ISTOP.EQ.1) GO TO 140
      JF=1
      DO 80 J=NLIMF,MAXF
      FF(JF)=FF(J)
   80 JF=JF+1
      DO 90 J=JF,MAXF
   90 FF(J)=0.
      JS=1
      DO 100 J=NLIMS,MAXS
      SF(JS)=SF(J)
  100 JS=JS+1
      DO 110 J=JS,MAXS
  110 SF(J)=0.
      JVS=1
      DO 120 J=NLIMVS,MAXVS
      VSF(JVS)=VSF(J)
  120 JVS=JVS+1
      DO 130 J=JVS,MAXVS
  130 VSF(J)=0.
      NLO=NSHIFT+1
  140 CALL SECOND (TIME)
      TIMPNL=TIMPNL+TIME-TIME0
      RETURN
C
C
C
  900 FORMAT (I10,24X,E12.5,F12.5)
      END
```

Table A2. Loader Map for HIRACC Program

```
LOAD MAP - HIRACC                                CYBER LOADER 1.1-424        07/11/77  23.37.29.       PAGE     1

FWA OF THE LOAD             111
LWA+1 OF THE LOAD         43546

TRANSFER ADDRESS -- HIRACC          11401

PROGRAM AND BLOCK ASSIGNMENTS.
```

BLOCK	ADDRESS	LENGTH	FILE	DATE	PROCSSR	VER	LEVEL	HARDWARE	COMMENTS
/XSUB/	111	16							
/WKX/	127	14							
/SUB1/	143	12							
/XPANEL/	155	5							
/XTIME/	162	4							
HIRACC	166	12404	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
SHAPE	12572	263	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
/XPOLEC/	13055	124							
POLEC	13201	220	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
OVRFAC	13421	111	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
RDFILE	13532	164	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
CONVFN	13716	230	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
PANEL	14146	467	LGO	07/11/77	FTN	4.5	414	666X I	OPT=1
/FCL.C./	14635	23							
/Q8.IO./	14660	131							
CORIO=	15011	44	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		COMMON CODED I/O ROUTINES AND CONSTANTS.
QQNTRY=	15211	8	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FCL INITIALIZATION ROUTINE.
ENDFIL=	15075	61	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		WRITE END OF LOGICAL FILE MARK.
FECNSK=	15156	41	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		INITIALIZE CONSTANTS.
FLTOUT=	15217	310	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		COMMON FLOATING OUTPUT CODE
FORSYS=	15527	601	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FORTRAN OBJECT LIBRARY UTILITIES.
INCOM=	16330	777	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		COMMON INPUT FORMATTING CODE
INPC=	16527	160	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FORMATTED READ FORTRAN RECORD.
KODER=	17027	456	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		OUTPUT FORMAT INTERPRETER.
OUTC=	17465	172	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FORMATTED WRITE FORTRAN RECORD.
ALOG	17657	73	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		COMPUTE COMMON AND NATURAL LOGARITHMS. OPT=ALL
EXP	17752	75	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		EXPONENTIAL FUNCTION. E TO POWER X. OPT=ALL.
SYSAID=	23347	1	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		LINK BETWEEN SYSAID AND INITIALIZATION CODE.
EOF	23350	16	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		TEST FOR END OF FILE STATUS.
FLTIN=	23066	154	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		COMMON FLOATING INPUT CONVERTER.
FMTAP=	28242	352	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		CRACK APLIST AND FORMAT FOR KODER/KRAKER.
FORUTL=	28614	16	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FCL MISC. UTILITIES.
GETFIT=	28632	42	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		LOCATE AN FIT GIVEN A FILE NAME.

Table A2. Loader Map for HIRACC Program (Cont.)

LOAD MAP - HIRACC

/IO.BUF./	20576	727						
INPB=	21123	314	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	BINARY READ FORTRAN RECORD.
KRAKER=	21437	406	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	PROCESS FORMATTED FORTRAN INPUT.
OUTB=	22045	203	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	BINARY WRITE FORTRAN RECORD.
OUTCOM=	22250	154	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	COMMON OUTPUT CODE
REWINB=	22424	37	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	POSITION FILE AT BEGINNING-OF-INFORMATION.
CLOCK=	22463	31	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	ACCESS SYSTEM CLOCKS FOR FORTRAN.
ACOSIN=	22514	71	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	COMPUTE THE INVERSE SINE OR COSINE OF X.
SYS=1ST	22605	62	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	MATH LIBRARY LINK TO ERROR MESSAGE PROCESSOR
XTOI=	22667	10	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	REAL TO INTEGER EXPONENTIATION.
XTOY=	22677	7	SL-FORTRAN	08/11/76	COMPASS	3.	2-414	REAL TO REAL EXPONENTIATION.
/CON.RM/	22706	6						
CIO.RM	22714	40	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/ABS.RM/	22754	10						
MOVE.RM	22764	64	SL-SYSIO	05/28/76	COMPASS	3.	75125	
NCT.RM	23050	233	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/JMPS.RM/	23303	11						
/MEMC.RM/	23314	3						
/OPES.FO/	23317	1						
/OPEN.FO/	23320	7						
OPEN.RM	23327	235	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/TERM.RM/	23564	1						
/PUT.FO/	23565	7						
PUT.SQ	23574	1362	SL-SYSIO	05/28/76	COMPASS	3.	75125	
WRR.SQ	25156	268	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/CLSF.FO/	25436	7						
CLSF.RM	25445	23	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/GET.RT/	25470	5						
STRT.SQ	25475	114	SL-SYSIO	05/28/76	COMPASS	3.	75125	
WEOR.SQ	25611	142	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/SKFL.FO/	25753	7						
SKFL.SQ	25762	47	SL-SYSIO	05/28/76	COMPASS	3.	75125	
ERR.RM	26031	404	SL-SYSIO	05/28/76	COMPASS	3.	75125	
CHKR.SQ	26435	7	SL-SYSIO	05/28/76	COMPASS	3.	75125	
GSIB.RM	26444	65	SL-SYSIO	05/28/76	COMPASS	3.	75125	
OPEN.SQ	26531	252	SL-SYSIO	05/28/76	COMPASS	3.	75125	
OPEX.SQ	27013	14	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/PUT.RT/	27027	11						
RLEO.RM	27040	42	SL-SYSIO	05/28/76	COMPASS	3.	75125	
CLSF.SQ	27102	132	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/CLSV.FO/	27234	7						
CLSV.SQ	27243	123	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/REW.FO/	27366	7						
REW.SQ	27375	31	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/GET.FO/	27426	7						

Table A2. Loader Map for HIRACC Program (Cont.)

```
LOAD MAP - HIRACC
/GET.RT/      27435       11
GET.SQ        27446     1335  SL-SYSIO      05/28/76 COMPASS  3. 75125
Z.SQ          30503      101  SL-SYSIO      05/28/76 COMPASS  3. 75125
Q.SQ          30604       50  SL-SYSIO      05/28/76 COMPASS  3. 75125
FSQ.SQ        30654      106  SL-SYSIO      05/28/76 COMPASS  3. 75125
SYS.RM        30762       37  SL-NUCLEUS    04/15/77 COMPASS  3. 2-414          PROCESS SYSTEM REQUEST.
 //           31021    12525

      .721 CP SECONDS            44100B CM STORAGE USED            70 TABLE MOVES
```

Table A3. Sample Output From HIRACC Program

```
    OCO AND NOH , 3550 TO 3650 FOR REPORT

OUTPUT FILE NO. =   10

SECANT =          1.00000

PRESS(MB) =    500.00000

TEMP(K) =      240.00

COLUMN DENSITY(MOLECULES/CM**2)

     H20  =  2.900E+18
     CO2  =  7.600E+18
      O3  = -0.
     N2O  = -0.
      CO  = -0.
     CH4  = -0.
      O2  = -0.

DV(CM-1) =           .0100

V1(CM-1) =     3550.0000

V2(CM-1) =     3650.0000

2*BOUND(CM-1) =   3.5438
```

Table A3. Sample Output From HIRACC Program (Cont.)

```
++++++++++++++++++++++++++++ 3558.4738       .149E-07   .158000    .066600    .000000     1
      769                     .19780E-02  3558.80000
      770                     .18811E-02  3558.81000
      771                     .17869E-02  3558.82000
      772                     .16573E-02  3558.83000
      773                     .16692E-02  3558.84000
      774                     .17411E-02  3558.85000
      775                     .18789E-02  3558.86000
      776                     .20963E-02  3558.87000
      777                     .24889E-02  3558.88000
      778                     .28353E-02  3558.89000
      779                     .34620E-02  3558.10000
      780                     .41280E-02  3558.11000
      781                     .46754E-02  3558.12000
      782                     .48183E-02  3558.13000
      783                     .44647E-02  3558.14000
      784                     .38362E-02  3558.15000
      785                     .32032E-02  3558.16000
     2416                     .56406E-01  3566.47000
     2417                     .66591E-01  3566.48000
     2418                     .78203E-01  3566.49000
     2419                     .94024E-01  3566.50000
     2420                     .11306E+00  3566.51000
     2421                     .13222E+00  3566.52000
     2422                     .15281E+00  3566.53000
     2423                     .16691E+00  3566.54000
     2424                     .17259E+00  3566.55000
     2425                     .16592E+00  3566.56000
     2426                     .15183E+00  3566.57000
     2427                     .13229E+00  3566.58000
     2428                     .11516E+00  3566.59000
     2429                     .98761E-01  3566.60000
     2430                     .87471E-01  3566.61000
     2431                     .77873E-01  3566.62000
     2432                     .70856E-01  3566.63000

   TIME        READ     CONVOLUTION        PANEL        V1          V2          DV      NVALUES
   5.754       .340         .719            .067     3558.0000   3566.6300    .0130     1664

 AVERAGE WIDTH =     .03868    NO. LINES =      1283    TOTAL NO. OF LINES=     1283
```

Table A3. Sample Output From HIRACC Program (Cont.)

```
------------------------ 3579.0810      .131E-07   .011750   .006441   .010003   1
------------------------ 3579.0075      .396E-07   .012030   .006578   .010300   1
    33                         .66222E-01  3566.64000
    34                         .62801E-01  3566.65000
    35                         .62345E-01  3566.66000
    36                         .62964E-01  3566.67000
    37                         .66502E-01  3566.68000
    38                         .73269E-01  3566.69000
    39                         .84911E-01  3566.70000
    40                         .10078E+00  3566.71000
    41                         .12546E+00  3566.72000
    42                         .16105E+00  3566.73000
    43                         .19919E+00  3566.74000
    44                         .22946E+00  3566.75000
    45                         .22841E+00  3566.76000
    46                         .19609E+00  3566.77000
    47                         .15594E+00  3566.78000
    48                         .11633E+00  3566.79000
    49                         .91763E-01  3566.80000
  2416                         .28074E-01  3590.47000
  2417                         .29933E-01  3590.48000
  2418                         .32079E-01  3590.49000
  2419                         .34602E-01  3590.50000
  2420                         .37426E-01  3590.51000
  2421                         .40465E-01  3590.52000
  2422                         .43434E-01  3590.53000
  2423                         .46314E-01  3590.54000
  2424                         .49843E-01  3590.55000
  2425                         .53757E-01  3590.56000
  2426                         .58293E-01  3590.57000
  2427                         .64084E-01  3590.58000
  2428                         .70955E-01  3590.59000
  2429                         .79524E-01  3590.60000
  2430                         .90559E-01  3590.61000
  2431                         .10363E+00  3590.62000
  2432                         .11919E+00  3590.63000

      TIME          REAC    CONVOLUTION        PANEL        V1            V2          DV      NVALUES
     6.638          .519          1.253         .142     3566.6400     3590.63[illegible]   .01[illegible]   24[illegible]

 AVERAGE WIDTH =     .03554    NO. LINES =        1000    TOTAL NO. OF LINES=     2283
```

Table A3. Sample Output From HIRACC Program (Cont.)

33	.13791E+00	3598.64000
34	.15801E+00	3598.65000
35	.17890E+00	3598.66000
36	.20826E+00	3598.67000
37	.23279E+00	3598.68000
38	.26232E+00	3598.69000
39	.30218E+00	3598.70000
40	.35899E+00	3598.71000
41	.43878E+00	3598.72000
42	.54916E+00	3598.73000
43	.70133E+00	3598.74000
44	.90392E+00	3598.75000
45	.11522E+01	3598.76000
46	.14011E+01	3598.77000
47	.15518E+01	3598.78000
48	.15187E+01	3598.79000
49	.13058E+01	3598.80000
2416	.12606E+00	3614.47000
2417	.16442E+00	3614.48000
2418	.21066E+00	3614.49000
2419	.25084E+00	3614.50000
2420	.27856E+00	3614.51000
2421	.25931E+00	3614.52000
2422	.21167E+00	3614.53000
2423	.16561E+00	3614.54000
2424	.12053E+00	3614.55000
2425	.10008E+00	3614.56000
2426	.81479E-01	3614.57000
2427	.68371E-01	3614.58000
2428	.59879E-01	3614.59000
2429	.52068E-01	3614.60000
2430	.48823E-01	3614.61000
2431	.45449E-01	3614.62000
2432	.45977E-01	3614.63000

TIME	READ	CONVOLUTION	PANEL	V1	V2	CV	NVALUES
7.354	.652	1.679	.227	3590.6400	3614.6300	.0100	24[illegible]

AVERAGE WIDTH = .03869 NO. LINES = 750 TOTAL NO. OF LINES= 3333

Table A3. Sample Output From HIRACC Program (Cont.)

33	.47769E-01	3614.64000
34	.52111E-01	3614.65000
35	.5[illegible]45E-01	3614.66000
36	.66956E-01	3614.67000
37	.83782E-01	3614.68000
38	.98963E-01	3614.69000
39	.10960E+00	36[illegible]4.70000
40	.10557E+00	3614.71000
41	.91775E-01	3614.72000
42	.74247E-01	[illegible]
43	.60445E-01	3614.74000
44	.49564E-01	3614.75000
45	.42435E-01	3614.76000
46	.37827E-01	3614.77000
47	.33496E-01	3614.78000
48	.31012E-01	3614.79000
49	.29256E-01	3614.80000
2416	.84396E-02	3638.47000
2417	.82575E-02	3638.48000
2418	.81237E-02	3638.49000
2419	.80196E-02	3638.50000
2420	.79461E-02	3638.51000
2421	.78965E-02	3638.52000
2422	.78536E-02	3638.53000
2423	.78321E-02	3638.54000
2424	.78339E-02	3638.55000
2425	.78597E-02	3638.56000
2426	.79104E-02	3638.57000
2427	.79878E-02	3638.58000
2428	.80904E-02	3638.59000
2429	.82192E-02	3638.60000
2430	.83739E-02	3638.61000
2431	.85584E-02	3638.62000
2432	.87747E-02	3638.63000

TIME	READ	CONVOLUTION	PANEL	V1	V2	DV	NVALUES
0.244	.827	2.222	.333	3614.6400	3638.6300	.0100	243[illegible]

AVERAGE WIDTH = .83852 NO. LINES = 1000 TOTAL NO. OF LINES= 4633

Table A3. Sample Output From HIRACC Program (Cont.)

33	.95241E-02	3638.64000
34	.92095E-02	3638.65000
35	.95974E-02	3638.66000
36	.99572E-02	3638.67000
37	.10378E-01	3638.68000
38	.10864E-01	3638.69000
39	.11436E-01	3638.70000
40	.12109E-01	3638.71000
41	.12900E-01	3638.72000
42	.13776E-01	3638.73000
43	.14811E-01	3638.74000
44	.16062E-01	3638.75000
45	.17562E-01	3638.76000
46	.19330E-01	3638.77000
47	.21392E-01	3638.78000
48	.23748E-01	3638.79000
49	.26422E-01	3638.80000
1153	.26749E-01	3649.84000
1154	.26530E-01	3649.85000
1155	.26384E-01	3649.86000
1156	.26197E-01	3649.87000
1157	.25795E-01	3649.88000
1158	.25089E-01	3649.89000
1159	.24387E-01	3649.90000
1160	.23580E-01	3649.91000
1161	.22965E-01	3649.92000
1162	.22460E-01	3649.93000
1163	.22045E-01	3649.94000
1164	.21727E-01	3649.95000
1165	.21481E-01	3649.96000
1166	.21297E-01	3649.97000
1167	.21176E-01	3649.98000
1168	.21100E-01	3649.99000
1169	.21113E-01	3650.00000

TIME	READ	CONVOLUTION	PANEL	V1	V2	DV	NVALUES
8.672	.912	2.484	.356	3638.6400	3650.0000	.0100	1137

AVERAGE WIDTH = .03745 NO. LINES = 368 TOTAL NO. OF LINES= 4401

Table A4. Data Cards for HIRACC Program

```
1     D2O AND HOH , 3550 TO 3650 FOR REPORT
   10  1.
 500.0E 06 240. E 06
 2.900E 18 7.600E 18 0.000E 00 0.000E 00 0.000E 00 0.000E 00 0.000E 00
 .01       3550.     3650.
99999
*EOR
```

Appendix B

A listing of a Fortran program to plot the results from HIRACC in transmission is given in Appendix B. This program, entitled TPLOT, was written for the CDC 6600 and the plotting functions are specific to that computer. This plot program is consistent with the sampling criterion and the interpolation methods described in this report. The four point Lagrange interpolation is used to generate three intermediate points for each output interval of HIRACC. The listing of the program, the output, and the input data, are given in Table B1. Two data cards are required: the first contains 30 characters of identification, and the second contains the upper and lower limits (cm^{-1}) of the wavenumber range and the distance in inches (DX) over which this wavenumber range is to be plotted.

Table B1. Listing of TPLOT Program

```
PROGRAM TPLOT       74/74    OPT=1                        FTN 4.5+414        07/12/77

            PROGRAM TPLOT(INPUT,OUTPUT,TAPE10)
            DIMENSION PROGID(3)
            COMMON Y(2500),XP(2500),YP(2500)
             DIMENSION XID(7),W(7),HMOL(7)
            HEQ=1H=
            READ 910, PROGID
            REWIND 10
            PRINT 910, PROGID
            CALL PLTID3 (PROGID,30.,0,11.0,0.8)
            READ 910, V1,V2,XSIZE
            IF (XSIZE.LT.1.0E-5) GO TO 100
            PRINT 930, V1,V2,XSIZE
             READ (10) (XID(I),I=1,7),SEC,P0,T0,(HMOL(M),M=1,7),
           &          (W(M),M=1,7),V0V,V1V,V2V
            DELY=0.5
            YT=10.
            YT=YT-DELY
             CALL SYMBOL(0.0,YT ,.15,XID, 0.0,70)
            YT=YT-DELY
             CALL SYMBOL(0.0,YT,0.15,5HSEC =,0.0,5)
             CALL NUMBER(1.0,YT,0.15,SEC,0.0,1)
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,0.15,11HPRESS (MB)=,0.0,11)
            CALL NUMBER(2.0,YT,0.15,P0,0.0,2)
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,0.15,9HTEMP (K)= ,0.0,9)
            CALL NUMBER(1.5,YT,0.15,T0, 0.0,1)
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,0.15,20HAMOUNTS (MOL/CM**2)  ,0.0,20)
             DO 20 M=1,7
            YT=YT-DELY
             RW=0.
            HIP=0.
             IF(W(M).LT.1.0E-23) GO TO 10
            IP=ALOG10(W(M))
            HIP=IP
            RW=W(M)/10.**IP
         10 CALL SYMBOL( 0.0,YT,.15,HMOL(M),0.0,6)
            CALL SYMBOL(1.0,YT,0.15,HEQ,0.0,1)
             CALL NUMBER(1.3,YT,.15,RW,0.0,3)
             CALL NUMBER(2.3,YT,.15,HIP,0.0,-1)
         20 CONTINUE
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,.15,10HDV(CM-1)=  ,0.0,10)
            CALL NUMBER(1.5,YT,0.15,V0V, 0.0,3)
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,0.15,10HV1(CM-1) =  ,0.0,10)
            CALL NUMBER(1.5,YT,0.15,V1V, 0.0,2)
            YT=YT-DELY
            CALL SYMBOL(0.0,YT,0.15,10HV2(CM-1) =  ,0.0,10)
            CALL NUMBER (1.5,YT,0.15,V2V,0 0,2)
             XT=7.0
             CALL PLOT(XT,0.0,-3)
            DX=(V2-V1)/XSIZE
            CALL AXIS (0.0,0.0,1H ,1,10.0,90.0,0.0,0.1,20.0)
            CALL AXIS (XSIZE,0.0,1H ,-1,10.0,90.0,0.0,0.1,20.0)
            CALL AXIS (0.0,10.0,1H ,1,XSIZE,0.0,V1,DX,20.0)
            CALL AXIS (0.0,0.0,10HWAVENUMBER,-10,XSIZE,0.0,V1,DX,20.0)
         50 READ (10) V1P,V2P,DV,NLIM
            IF (EOF(10)) 100,60
         60 LIMHI=NLIM+4
            IF (V1P.GT.V2) GO TO 100
            PRINT 920, V1P,V2P,DV,NLIM,LIMHI
            READ (10) (Y(I),I=5,LIMHI)
            IF (V2P.LT.V1) GO TO 50
            ILO=3
            IHI=ILO+605
            DO 70 I=5,LIMHI
            OAV=Y(I)
            Y(I)=0.
            IF (OAV.LT.20.0) Y(I)=EXP(-OAV)
```

Table B1. Listing of TPLOT Program (Cont.)

```
PROGRAM TPLOT

          CONTINUE
          IF (V1P.GT.V1) GO TO 80
          ILO=(V1-V1P)/DV+5.001
          IHI=ILO+600
          IF (IHI.GE.LIMHI) IHI=LIMHI-1
   80     IF (V2P.LT.V2) GO TO 90
          LIMHI=(V2-V1P)/DV+5.001
          IF (LIMHI.LT.600) IHI=LIMHI-1
   90     CALL LPP (ILO,IHI,V1P,V1,DX,DV)
          ILO=IHI
          IHI=ILO+600
          IF (IHI.LT.LIMHI) GO TO 90
          IHI=LIMHI-1
          IF (ILO.LT.(LIMHI-1)) GO TO 90
          Y(1)=Y(LIMHI-3)
          Y(2)=Y(LIMHI-2)
          Y(3)=Y(LIMHI-1)
          Y(4)=Y(LIMHI)
          IF (LIMHI.LT.NLIM) GO TO 100
          GO TO 50
  100     CALL PLOT (XSIZE+3.0,0.0,-3)
          CALL ENDPLT
          STOP
C
C
  900     FORMAT (5(I12,F10.6))
  910     FORMAT (3A10)
  920     FORMAT (3F12.3,2I10)
  930     FORMAT (4F10.3,4I5)
          END
```

```
SUBROUTINE LPP

          SUBROUTINE LPP (ILO,IHI,V1P,V1,DX,DV)
          COMMON Y(2500),XP(2500),YP(2500)
          PRINT 910, ILO,IHI,V1P
          DV1=DV/4.
          DV2=DV1+DV1
          DV3=DV2+DV1
          X00=-7./128.
          X01=105./128.
          X02=35./128.
          X03=-5./128.
          X10=-1./16.
          X11=9./16.
          IP=1
          IMAX=IHI-1
          DO 10 I=ILO,IMAX
          XP(IP)=V1P+DV*FLOAT(I-5)
          XP(IP+1)=XP(IP)+DV1
          XP(IP+2)=XP(IP)+DV2
          XP(IP+3)=XP(IP)+DV3
          YP(IP)=Y(I)
          YP(IP+1)=X00*Y(I-1)+X01*Y(I)+X02*Y(I+1)+X03*Y(I+2)
          YP(IP+2)=X10*(Y(I-1)+Y(I+2))+X11*(Y(I)+Y(I+1))
          YP(IP+3)=X03*Y(I-1)+X02*Y(I)+X01*Y(I+1)+X00*Y(I+2)
          IP=IP+4
   10     CONTINUE
          XP(IP)=V1P+DV*FLOAT(IHI-5)
          YP(IP)=Y(IHI)
          CALL LINE (XP,YP,IP,1,0,1,V1,DX,0.0,0.1,0.00)
          RETURN
C
C
  900     FORMAT (5(F12.3,F10.6))
  910     FORMAT (2I10,F12.3,* ILO,IHI,V1P*)
          END
```

Table B2. Loader Map for TPLOT Program

LOAD MAP - TPLOT   CYBER LOADER 1.1-428   07/12/77 10.31.45.   PAGE   1

FWA OF THE LOAD   111
LWA+1 OF THE LOAD   50161

TRANSFER ADDRESS -- TPLOT   6262

PROGRAM AND BLOCK ASSIGNMENTS.

BLOCK	ADDRESS	LENGTH	FILE	DATE	PROCSSR	VER	LEVEL	HARDWARE	COMMENTS
TPLOT	111	7177	LGO	07/12/77	FTN	4.5	414	666X I	OPT=1
LP?	7310	202	LGO	07/12/77	FTN	4.5	414	666X I	OPT=1
/NAME/	7512	6							
/MANIT/	7520	1							
/C4EXP/	7521	1							
/TAGIT/	7522	1							
/SAVONG/	7523	5							
PLTFD3	7530	171	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
BLOXIT	7721	54	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
PLOT	7775	325	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
ERRPLT	10322	235	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
FACTOR	10557	16	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
SYMBOL	10575	387	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
PLOTDO	11164	432	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
PLOCODE	11536	425	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
ENDPLT	12163	160	UL-PEN	10/14/75	FTN	4.5	414	666X I	OPT=2
DOTX	12343	41	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
PLOTTX	12404	23	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
WHERE	12427	52	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
CHEXIT	12501	11	UL-PEN	10/06/76	COMPASS	3.	2-414		
LINE	12512	310	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
NUMBER	13022	233	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
NEWPEN	13255	66	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
PLOTS	13343	75	UL-PEN	10/06/76	FTN	4.5	414	666X I	OPT=2
BUFF	13440	467	UL-PEN	10/06/75	COMPASS	3.	2-414		
ASGNTS	14127	4	UL-PEN	10/06/76	COMPASS	3.	2-414		
AXIS	14133	576	UL-PEN	10/14/76	FTN	4.5	414	666X I	OPT=2
/FCL.C./	14731	23							
/Q8.IO./	14754	131							
COMIO=	15105	64	SL-FORTRAN	10/11/76	COMPASS	3.	2-414		COMMON CODED I/O ROUTINES AND CONSTANTS.
Q8NTRY=	15165	6	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		FCL INITIALIZATION ROUTINE.
EOF	15171	16	SL-FORTRAN	08/11/76	COMPASS	3.	2-414		TEST FOR END OF FILE STATUS.

Table B2. Loader Map for TPLOT Program (Cont.)

LOAD MAP - TPLOT

FLTIN=	15207	154	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMMON FLOATING INPUT CONVERTER.
FMTAP=	15363	352	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	CRACK APLIST AND FORMAT FOR KODER/KRAKER.
FORUTL=	15735	16	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	FCL MISC. UTILITIES.
GETFIT=	15753	42	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	LOCATE AN FIT GIVEN A FILE NAME.
/IO.BUF./	16015	227					
INPB=	16244	314	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	BINARY READ FORTRAN RECORD.
KRAKER=	16560	406	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	PROCESS FORMATTED FORTRAN INPUT.
OUTC=	17166	172	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	FORMATTED WRITE FORTRAN RECORD.
SYSTEMC	17360	372	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	EXTENDED ERROR HANDLING OPTION.
CLOCK=	17752	31	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	ACCESS SYSTEM CLOCKS FOR FORTRAN.
GOTOER=	20033	14	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMPUTED GO TO ERROR PROCESSOR.
ALOG	20017	73	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMPUTE COMMON AND NATURAL LOGARITHMS. OPT=ALL
EXP	20112	75	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	EXPONENTIAL FUNCTION. E TO POWER X. OPT=ALL.
SINCOS=	20207	66	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	TRIGONOMETRIC SINE OR COSINE OF X. OPT=ALL.
SYSAID=	20275	1	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	LINK BETWEEN SYS=AID AND INITIALIZATION CODE.
FECNSK=	20276	41	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	INITIALIZE CONSTANTS.
FLTOUT=	20337	310	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMMON FLOATING OUTPUT CODE
FORSYS=	20647	601	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	FORTRAN OBJECT LIBRARY UTILITIES.
INCOM=	21450	277	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMMON INPUT FORMATTING CODE
INPC=	21747	160	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	FORMATTED READ FORTRAN RECORD.
KODER=	22127	456	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	OUTPUT FORMAT INTERPRETER.
OUTCOM=	22605	154	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	COMMON OUTPUT CODE
REWIND=	22761	37	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	POSITION FILE AT BEGINNING-OF-INFORMATION.
SYSTEM	23020	21	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	USER CALLABLE ERROR PROCESSOR.
SYS=1ST	23041	62	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	MATH LIBRARY LINK TO ERROR MESSAGE PROCESSOR.
XTOI=	23123	10	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	REAL TO INTEGER EXPONENTIATION.
XTOY=	23133	7	SL-FORTRAN	08/11/76	COMPASS	3. 2-414	REAL TO REAL EXPONENTIATION.
/CIO.PM/	23142	6					
CIO.RM	23150	40	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/ABS.PM/	23210	10					
MOVE.PM	23220	64	SL-SYSIO	05/28/76	COMPASS	3. 75125	
GET.RM	23304	233	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/JMPS.RM/	23537	11					
/MEMC.RM/	23550	3					
/OPES.FO/	23553	1					
/OPEN.FO/	23554	7					
OPEN.RM	23563	235	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/PJT.PT/	24020	11					
RLEQ.PM	24031	42	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/CLSF.FO/	24073	7					
CLSF.SQ	24102	132	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/CLSV.FO/	24234	7					
CLSV.SQ	24243	123	SL-SYSIO	05/28/76	COMPASS	3. 75125	
/REW.FO/	24366	7					
REW.SQ	24375	31	SL-SYSIO	05/28/76	COMPASS	3. 75125	

Table B2. Loader Map for TPLOT Program (Cont.)

LOAD MAP - TPLOT

/TERM.RM/	24426	1						
/GET.FO/	24427	7						
/GET.ST/	24436	5						
/GET.PT/	24443	11						
GET.SQ	24454	1035	SL-SYSIO	05/28/76	COMPASS	3.	75125	
Z.SC	25511	101	SL-SYSIO	05/28/76	COMPASS	3.	75125	
U.SQ	25612	50	SL-SYSIO	05/28/76	COMPASS	3.	75125	
FSU.SQ	25662	106	SL-SYSIO	05/28/76	COMPASS	3.	75125	
ERR.RM	25770	404	SL-SYSIO	05/28/76	COMPASS	3.	75125	
CWAR.SQ	26374	7	SL-SYSIO	05/28/76	COMPASS	3.	75125	
OSUB.PM	26403	65	SL-SYSIO	05/28/76	COMPASS	3.	75125	
OPEN.SQ	26470	262	SL-SYSIO	05/28/76	COMPASS	3.	75125	
OPEX.SQ	26752	14	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/PUT.FO/	26766	7						
PUT.RM	26775	2	SL-SYSIO	05/28/76	COMPASS	3.	75125	
PUT.SQ	26777	1362	SL-SYSIO	05/28/76	COMPASS	3.	75125	
WAR.SQ	30361	260	SL-SYSIO	05/28/76	COMPASS	3.	75125	
CLSF.RM	30641	23	SL-SYSIO	05/28/76	COMPASS	3.	75125	
BTRT.SQ	30664	114	SL-SYSIO	05/28/76	COMPASS	3.	75125	
WEOI.SQ	31060	142	SL-SYSIO	05/28/76	COMPASS	3.	75125	
/SKFL.FO/	31142	7						
SKFL.SQ	31151	47	SL-SYSIO	05/28/76	COMPASS	3.	75125	
RECOVR	31220	156	SL-NUCLEUS	04/15/77	COMPASS	3.	2-414	REPRIEVE INTERFACE
SYS.RP	31406	37	SL-NUCLEUS	04/15/77	COMPASS	3.	2-414	PROCESS SYSTEM REQUEST.
//	31445	16514						

.070 CP SECONDS   44500B CM STORAGE USED   67 TABLE MOVES

Table B3. Sample Output From TPLOT Program

```
CLOUGH LORENTZ(40) JULY 11,77
 3550.000  3650.050    40.000
   3550.000     3566.630          .010        1664         1668
          5          605    3550.000 ILO,INI,V1P
        605         1205    3550.000 ILO,INI,V1P
       1205         1667    3550.000 ILO,INI,V1P
   3566.640     3590.630          .010        2400         2404
          3          603    3556.640 ILO,INI,V1P
        603         1203    3566.640 ILO,INI,V1P
       1203         1803    3566.640 ILO,INI,V1P
       1803         2403    3566.640 ILO,INI,V1P
   3590.640     3614.630          .010        2400         2404
          3          603    3590.640 ILO,INI,V1P
        603         1203    3590.640 ILO,INI,V1P
       1203         1803    3590.640 ILO,INI,V1P
       1803         2403    3590.640 ILO,INI,V1P
   3614.640     3638.630          .010        2400         2404
          3          603    3614.640 ILO,INI,V1P
        603         1203    3614.640 ILO,INI,V1P
       1203         1803    3614.640 ILO,INI,V1P
       1803         2403    3614.640 ILO,INI,V1P
   3638.640     3658.000          .010        1137         1141
          3          603    3638.640 ILO,INI,V1P
        603         1140    3638.640 ILO,INI,V1P


END OF PLOTS.
```

Table B4. Data Cards for TPLOT Program

```
CLOUGH LORENTZ(48) JULY 11,77
 3558.    3658.     48.
```